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STRUCTURE FILE UPDATES: 4 JUL 2005 HIGHEST RN 853727-85-2 DICTIONARY FILE UPDATES: 4 JUL 2005 HIGHEST RN 853727-85-2

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que 123

L1 STR

2 7 13

18 CY 1 C 3 C 8 12 C C 14

6 C 4 N G1 11 @17 C 0 15

5 10 16

VAR G1=S/N/C/17 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE L14 STR

VAR G1=S/N/C/17 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L16 1063 SEA FILE=REGISTRY SSS FUL L14

L23 77 SEA FILE=REGISTRY SUB=L16 SSS FUL L1

100.0% PROCESSED 1063 ITERATIONS 77 ANSWERS

SEARCH TIME: 00.00.01

=> d ide can 1115

L115 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-42-7 REGISTRY

ED Entered STN: 29 Nov 2000

CN 1H-Pyrrole-2-carbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile

CN NSP 989

CN Tanaproget

FS 3D CONCORD

MF C16 H15 N3 O S

SR CA

LC STN Files: ADISINSIGHT, CA, CAPLUS, IMSDRUGNEWS, IMSRESEARCH, PHAR, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## 4 REFERENCES IN FILE CA (1907 TO DATE)

jan delaval - 5 july 2005

## 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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REFERENCE
            1: 142:266842
REFERENCE
            2:
               140:71530
REFERENCE
            3: 140:53469
REFERENCE
               133:350228
            4:
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L1
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L2
     FILE 'HCAPLUS' ENTERED AT 07:20:57 ON 05 JUL 2005
L3
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                E FONSOME A/AU
                E FENSOME A/AU
L4
             37 S E3, E6, E7
                E HARRISON D/AU
L5
            123 S E3, E8, E114-E116, E118
                E WINNEKER R/AU
L6
             59 S E4-E7
                E ZHANG P/AU
L7
            307 S E3,E17
                E ZHANG PU/AU
            136 S E3, E24, E25
L8
                E ZHANG P/AU
            694 S E3-E20
L9
                E KERN J/AU
            203 S E3, E5, E29-E31, E34
L10
                E TEREFENKO E/AU
L11
             24 S E4-E7
                E WYETH/PA, CS
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           4429 S E4-E7 OR WYETH?/PA,CS
L12
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L13
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L14
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L15
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L16
           1063 S L14 FUL
                SAV L16 KWON601/A
L17
             60 S L13 AND L16
L18
             24 S L13 NOT L17
L19
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L20
             14 S L18 NOT L19
L21
             4 S L20 AND NCOC3-C6/ES
             14 S L19, L21
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L23
             77 S L1 FUL SUB=L16
                SAV L23 KWON601A/A
L24
             17 S L23 NOT L17
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L27
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L28
              6 S L22
              13 S'L27, L28
L29
L30
               6 S L29 AND L3-L12
                 E HIRSUTISM/CT
                 E E3+ALL
L31
           968 S E4
L32
            1517 S E4,E5/BI
                 E HYPERTRICH
L33
             134 S E4-E7
                 E HIRSUT
L34
               1 S L29 AND L31-L33
L35
               1 S L29 AND HIRSUT?
                 E ACNE/CT
L36
            3716 S E3-E8
                 E E3+ALL
L37
            3741 S E6+NT
L38
            6082 S E6,E7/BI
L39
            243 S PIMPL?
L40
            6272 S ACNE?
                 E ACNE/CT
                 E E6+ALL
L41
             301 S E2
L42
               1 S L29 AND L36-L41
                E ECZEMA/CT
L43
            2222 S E3,E4
                 E E3+ALL
L44
            2222 S E9
L45
            3655 S E9,E10/BI
L46
               1 S L29 AND ECZEM?
L47
               1 S L3, L34, L35, L42, L46
                 E SKIN/CT
                 E E3+ALL
L48
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L49
         124391 S E6+PFT, RT
                 E E37+ALL
L50
         139455 S E5+OLD, NT, PFT, RT
                 E E181+ALL
L51
         155162 S E3+OLD, NT, PFT, RT
L52
         142584 S E13+OLD, NT, PFT, RT
          16036 S E16+OLD, NT, PFT, RT
L53
               2 S L29 AND L48-L53
L54
                 E HAIR/CT
L55
          52596 S E3+OLD, NT, PFT, RT
L56
          52664 S E43+OLD, NT, PFT, RT
L57
          20289 S E86+OLD, NT, PFT, RT
                 E SKIN CONDITION/CT
                 E E4+ALL
L58
           1145 S E2
L59
               1 S L29 AND L55-L58
L60
               2 S L47, L54, L59
L61
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                 E PROGESTERONE RECEPTOR/CT
L62
           3809 S E8-E14
                 E E8+ALL
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L63
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L64
            9236 S E11+PFT, RT
L65
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                 E ENDOMETRIOSIS/CT
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L66
            1849 S E2
L67
            2470 S E1/BI
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                 E E3+ALL
L68
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             655 S E1/BI
L69
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L70
            2319 S E2/BI
                 E ENDOMETRIUM/CT
                 E E3+ALL
L71
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            647 S E6, E7
L72
L73
            1424 S E9, E10
L74
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L75
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L76
            386 S E18, E19
L77
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L78
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L79
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          18487 S E54+OLD, NT
L80
L81
          14597 S E67+OLD, NT
                 E BREAST/CT
                 E E3+ALL
                E E2+ALL
L82
          63582 S E3+OLD, NT
          50658 S E9+OLD, NT
L83
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L84
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L85
          47677 S E53+OLD, NT
                 E COLON/CT
                 E E3+ALL
L86
          31294 S E1,E2
                 E COLON, DISEASE/CT
                 E E2+ALL
          18615 S E2
L87
                 E PROSTATE/CT
L88
              26 S E3+OLD, NT
          32483 S E18+OLD, NT
L89
L90
          32840 S E53+OLD, NT, PFT, RT OR E57+OLD, NT, PFT, RT
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                 E E2+ALL
L91
          41881 S E3+OLD, NT OR E15+OLD, NT
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                 E E3+ALL
L92
            668 S E2,E3
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                 E UTERINE MYOMETRIAL FIBROID/CT
                 E MYOMETRIAL FIBROID/CT
                 E E5+ALL
L93
           3124 S E2
                 E UTERINE FIBROID/CT
                 E FIBROID/CT
                 E E4+ALL
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722 S E2
L94
L95
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              9 S L60, L65, L95
L96
                E UTERUS, NEOPLASM/CT
L97
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                E PROSTATE, NEOPLASM/CT
                E PROSTATIC NEOPLASM/CT
                E E4+ALL
L98
          19786 S E2+OLD, NT
                E PITUITARY NEOPLASM/CT
                E E3+ALL
L99
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                E BREAST NEOPLASM/CT
                E E3+ALL
L100
          47677 S E2+OLD, NT
                E OVARY, NEOPLASM/CT
L101
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                E COLON, NEOPLASM/CT
                E COLON NEOPLASM/CT
                E E4+ALL
          18615 S E2
L102
L103
              2 S L29 AND L97-L102
              9 S L96, L103
L104
                E CARCINOMA/CT
L105
         108005 S E3+OLD, NT
              1 S L29 AND L105
L106
                E ANTIPROGEST/CT
                E E4+ALL
L107
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L108
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L109
             9 S L30,L109
L110
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L111
              7 S L110 AND L111
L112
              4 S L111 NOT L112
L113
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L114
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L115
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L116
L117
              3 S L116 AND (PD<=20020625 OR PRD<=20020625 OR AD<=20020625)
              9 S L116, L117, L112
L118
              9 S L118 AND L3-L12, L27-L113
L119
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This file contains CAS Registry Numbers for easy and accurate substance identification.

## => d l119 all fhitstr tot

L119 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:219714 HCAPLUS

DN 142:266842

ED Entered STN: 11 Mar 2005

TI Partially absorbable fiber-reinforced composites for controlled drug delivery

IN Shalaby, Shalaby W.

PA USA

SO U.S. Pat. Appl. Publ., 9 pp., Cont.-in-part of U.S. Ser. No. 860,677. CODEN: USXXCO

DT Patent

LA English

IC ICM A61F002-00

INCL 424426000

CC 63-6 (Pharmaceuticals)

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
ΡI	US 2005053639	A1	20050310	US 2004-935808	20040908		
	US 2004265355	A1	20041230	US 2004-860677	20040603		
PRAI	US 2003-482898P	P	20030626				
	US 2004-860677	A2	20040603				

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2005053639	ICM INCL	A61F002-00 424426000
US 2005053639	NCL ECLA	424/426.000 A61L031/12D10; A61L031/16
US 2004265355	NCL ECLA	424/426.000 A61L031/12D10; A61L031/16

This invention describes a partially absorbable, fiber-reinforced composite in the form of a ring, or a suture-like thread, with modified terminals for use as a controlled delivery system of at least one bioactive agent, wherein said composite comprising an absorbable fiber construct capable of providing time-dependent mech. properties of a biostable elastomeric matrix containing an absorbable microparticulate ion-exchanger to modulate the release of the bioactive agent(s) for a desired period(s) of time at a specific biol. site, such as a vaginal canal, peritoneal cavity, scrotum, prostate gland, an ear loop, or s.c. tissue. Such drug delivery systems can be used for the local administration of at least one bioactive agent, including those used as contraceptive, antimicrobial, anti-inflammatory and/or antiviral agents as well as for cancer treatment. For example, an antimicrobial intravaginal

ring was prepared containing a two-component Silastic matrix comprising Component A 2.3 g and Component B 2.3 g, fiber-reinforcing construct, i.e., suture made of segmented L-lactide-trimethylene carbonate copolymer 300 mg, polyglycolide cation-exchanging microparticulate 7 mg, metronidazole 137 mg, and D&C Violet #2 3.8 mg.

- ST polymer fiber composite controlled delivery system; elastomer matrix ion exchanger microparticle fiber controlled release
- IT Silicone rubber, biological studies
  RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
  (Silastic, matrix; partially absorbable fiber-reinforced composites for controlled drug delivery)

- IT Polyesters, biological studies
  RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
  (caprolactone-based; partially absorbable fiber-reinforced composites for controlled drug delivery)
- IT Drug delivery systems
   (controlled-release; partially absorbable fiber-reinforced composites
   for controlled drug delivery)
- IT Silicone rubber, biological studies
  RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
  (di-Me, matrix; partially absorbable fiber-reinforced composites for controlled drug delivery)
- IT Parturition (inducers; partially absorbable fiber-reinforced composites for controlled drug delivery)
- IT Polyester fibers, biological studies
  RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
  (lactone-based; partially absorbable fiber-reinforced composites for controlled drug delivery)
- IT Ear (loop; partially absorbable fiber-reinforced composites for controlled drug delivery to specific biol. site)
- IT Cation exchangers
  Ion exchangers
  (microparticles; partially absorbable fiber-reinforced composites for controlled drug delivery)
- IT Antibodies and Immunoglobulins
  RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
  (monoclonal; partially absorbable fiber-reinforced composites for controlled drug delivery)
- IT Infection (parasitism, treatment of; partially absorbable fiber-reinforced composites for controlled drug delivery)
- IT Analgesics Anesthetics

Anti-inflammatory agents Antimicrobial agents Antipsychotics Antitumor agents Antiviral agents Composites Contraceptives (partially absorbable fiber-reinforced composites for controlled drug delivery) Antiprogestins IT Hormones, animal, biological studies Synthetic polymeric fibers, biological studies RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (partially absorbable fiber-reinforced composites for controlled drug delivery) ΙT Muscle Peritoneum Prostate gland Skin Vagina (partially absorbable fiber-reinforced composites for controlled drug delivery to specific biol. site) IT Urethane rubber, biological studies RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (polyether-, matrix; partially absorbable fiber-reinforced composites for controlled drug delivery) IT Vaccines (recombinant; partially absorbable fiber-reinforced composites for controlled drug delivery) TT Connective tissue (s.c.; partially absorbable fiber-reinforced composites for controlled drug delivery to specific biol. site) IT Reproductive organ (scrotum; partially absorbable fiber-reinforced composites for controlled drug delivery to specific biol. site) IT Contraceptives (spermicidal; partially absorbable fiber-reinforced composites for controlled drug delivery) ITMedical goods (sutures; partially absorbable fiber-reinforced composites for controlled drug delivery) IT Mycosis Ovary, neoplasm (treatment of; partially absorbable fiber-reinforced composites for controlled drug delivery) IT Immunomodulators (vaccines; partially absorbable fiber-reinforced composites for controlled drug delivery) IT Drug delivery systems (vaginal, ring; partially absorbable fiber-reinforced composites for controlled drug delivery) ITInfection (viral, treatment of; partially absorbable fiber-reinforced composites for controlled drug delivery) 41706-81-4P, ε-Caprolactone-glycolide copolymer ITRL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (coating; partially absorbable fiber-reinforced composites for controlled drug delivery) 140397-67-7, L-Lactide-trimethylene carbonate block copolymer

IT

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (fiber; partially absorbable fiber-reinforced composites for controlled drug delivery)

IT 26009-03-0P, Polyglycolide 26202-08-4P, Polyglycolide RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(microparticulate; partially absorbable fiber-reinforced composites for controlled drug delivery)

IT 7631-86-9, Silica, biological studies

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (microparticulate; partially absorbable fiber-reinforced composites for controlled drug delivery)

IT 50-81-7, Ascorbic acid, biological studies 58-22-0, Testosterone 299-29-6, Iron gluconate 443-48-1, Metronidazole 13598-36-2D, Phosphonic acid, alkylidenebis-derivs. 304853-42-7, Tanaproget

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (partially absorbable fiber-reinforced composites for controlled drug delivery)

IT 9016-00-6, Polydimethylsiloxane 31900-57-9, Polydimethylsiloxane RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (rubber, matrix; partially absorbable fiber-reinforced composites for controlled drug delivery)

IT 304853-42-7, Tanaproget

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (partially absorbable fiber-reinforced composites for controlled drug delivery)

RN 304853-42-7 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & H \\ N & N \\ NC & Me \\ Me & Me \\ \end{array}$$

L119 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:658042 HCAPLUS

ED Entered STN: 15 Aug 2004

TI Synthesis and SAR of novel, 6-aryl-1,4-dihydrobenzo[d][1,3]oxazine-2-thiones as progesterone receptor modulators leading to the potent and selective non-steroidal PR agonist Tanaproget

AU Fensome, Andrew; Chopra, Rajiv; Cohen, Jeff; Collins, Mark A.; Hudak, Valerie; Malakian, Karl; Olland, Andrea; Svenson, Kristine; Terefenko, Eugene A.; Unwalla, Ray J.; Wilhelm, James, M.; Wolfrom, Scott; Zhu, Yuan; Zhang, Zhiming; Zhang, Puwen; Winneker, Richard C.; Wrobel, Jay

CS Chemical and Screening Sciences, Wyeth Research, Collegeville, PA, 19426, USA

SO Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, United States, August 22-26, 2004 (2004), MEDI-178 Publisher: American Chemical Society, Washington, D. C. CODEN: 69FTZ8

DT Conference; Meeting Abstract

LA English Previously, we described the synthesis and SAR of a novel series of AB progesterone receptor (PR) antagonists based upon the 6-aryl-1,4-dihydrobenzo[d][1,3]oxazin-2-one ring system (e.g. 1, IC50 = 30 nM). More recently, we described the conversion of this class into potent PR agonists by the incorporation of sulfur to give 6-aryl-1,4-dihydrobenzo[d][1,3]oxazine-2-thiones (e.g. 2, EC50 = 0.4 nM). We also found in the antagonist series that we could make functional agonists by changing the 6-aryl group to a 2-cyanopyrrole (e.g. 3, EC50 = 1.1 nM). It was then apparent that combining these features would increase potency. Incorporation of the 5'-cyano-2'-pyrrole moiety onto the 1,4-dihydrobenzo[d][1,3]oxazine-2-thione core produced the highly potent and selective non-steroidal PR receptor agonist 4, tanaproget (EC50 = 0.12 nM). In this presentation, we will demonstrate that tanaproget represents a potential first-in-class nonsteroidal PR agonist for contraception. Addnl. SAR, biol. activity and structural information from a tanaproget/hPR-LBD co-crystal structure will be presented. L119 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN ΑN 2004:2847 HCAPLUS DN 140:71530 ED Entered STN: 02 Jan 2004 Use of cyclothiocarbamate derivatives as selective androgen antagonists in ΤI contraception, hormone replacement therapy and in treatment of other hormone-related conditions Fensome, Andrew; Grubb, Gary; Harrison, Diane Deborah; IN Winneker, Richard Craig; Zhang, Puwen; Kern, Jeffrey Curtis; Terefenko, Eugene Anthony PA Wyeth, John, and Brother Ltd., USA PCT Int. Appl., 79 pp. SO CODEN: PIXXD2 DT Patent LA English IC ICM C07D CC 2-4 (Mammalian Hormones) Section cross-reference(s): 1, 28, 63 FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. ----------\_\_\_\_\_ ---------PΙ WO 2004000801 A2 20031231 WO 2003-US19751 20030623 <--20040325 WO 2004000801 Α3 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG CA 2003-2489847 CA 2489847 20031231 20030623 <--AA US 2004006060 A1 20040108 US 2003-601481 20030623 <--

AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

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BR 2003-12024

EP 2003-761263

20030623 <--

20030623 <--

20050322

20050323

20020625

20030623

BR 2003012024

EP 1515725

PRAI US 2002-391871P

WO 2003-US19751

Α

A2

Р

W

PAT	TENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
WO	2004000801	ICM	C07D	
WO	2004000801	ECLA	A61K031/426+M; A61K031/536; A61K031/536+M; A61K031/54+M; A61K031/554; A61K031/554+M	A61K031/54;
US	2004006060	NCL ECLA	514/211.030; 514/227.200; 514/369.000 A61K031/426; A61K031/426+M; A61K031/536+M; A61K031/54+M; A61K031/554; A61K031/554+M	A61K031/54;
OS GI	MARPAT 140:	71530		

AB The present invention provides methods of inducing contraception which includes delivering to a female a composition containing cyclothiocarbamates (shown

as I and II; variables defined below; e.g. III) or tautomers thereof, in a regimen which involves delivering ≥1 of a selective estrogen receptor modulator. Methods of providing hormone replacement therapy and for treating carcinomas, dysfunctional bleeding, uterine leiomyomata, endometriosis, and polycystic ovary syndrome is provided which includes delivering I or II and a selective estrogen receptor modulator are also described. III (5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile) showed significant antagonistic activity towards androgens in L929 cells over a nine point dose response (IC50 = 109 nM) and only marginal agonistic activity at the maximum concentration tested (i.e., 10 nM). Although neither I nor II nor the methods of preparation are claimed, 6 example prepns. are included. example, 1-methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'cyclobutan]-6-yl]-1H-pyrrole-2-carbonitrile was prepared in 5 steps (32, 58, 52, 79, and 49 % yields, resp.) starting from phenylcarbamic acid tert-Bu ester, cyclobutanone and tBuLi in Et2O and involving intermediates tert-Bu [2-(1-hydroxycyclobutyl)phenyl]carbamate, spiro[3,1-benzoxazine-4,1'cyclobutan] -2 (1H) -one, 6-bromospiro[3,1-benzoxazine-4,1'-cyclobutan] -2 (1H) one, and 1-methyl-5-[2-oxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'cyclobutan]-6-yl]-1H-pyrrole-2-carbonitrile. For I: R1 and R2 = H, (un) substituted C1 to C6 alkyl, (un) substituted C2-C6 alkenyl, (un) substituted C2-C6 alkynyl, (un) substituted C3-C8 cycloalkyl, (un) substituted aryl, (un) substituted C-based heterocyclic ring having in its backbone 1-3 heteroatoms, CORA, and NRBCORA; or R1 and R2 are fused to form a ring (a), (b) and (c), wherein said ring is (un)substituted by 1-3 substituents H and C1 to C3 alkyl ((a) a C-based 3 to 8 membered saturated spirocyclic ring; (b) a C-based 3 to 8 membered spirocyclic ring having

≥1 C-C double bonds; and (c) a 3 to 8 membered spirocyclic ring having in its backbone 1-3 heteroatoms O, S and N). R3 = H, OH, NH2, (un) substituted C1 to C6 alkyl, (un) substituted C3-C6 alkenyl, (un) substituted alkynyl, and CORC; R4 = H, halogen, CN, NO2, (un) substituted C1 to C6 alkyl, C1 to C6 alkoxy, C1 to C6 aminoalkyl; R5 = an X/Y/Z-substituted Ph or a five or six membered C-based heterocyclic ring having in its backbone 1-3 heteroatoms O, S, SO, SO2, and NR6 and having one or two independent substituents H, halogen, CN, NO2, (un) substituted C1 to C4 alkyl, (un) substituted C1 to C3 alkoxy, (un) substituted C1 to C3 aminoalkyl, (un) substituted C1 to C3 perfluoroalkyl, (un)substituted 5 or 6 membered C-based heterocyclic ring having in its backbone 1-3 heteroatoms, (un)substituted C1 to C3 thioalkyl, CORF, and NRGCORF; Q1 = S, NR7, and CR8R9; addnl. details are given in the claims. For II: R1' = Me, Et, trifluoromethyl; R2' = Me, Et, trifluoromethyl; or R1' and R2' are joined to form a spirocyclic ring containing 3 to 7 C atoms; and R3 =C1 to C4 alkyl; other variables are as for

ST cyclothiocarbamate prepn androgen antagonist contraceptive hormone replacement therapy compn; antitumor agent carcinoma cyclothiocarbamate prepn; dysfunctional bleeding cyclothiocarbamate therapy; uterine leiomyomata cyclothiocarbamate therapy; endometriosis cyclothiocarbamate therapy; polycystic ovary syndrome cyclothiocarbamate therapy; benzoxazinone prepn androgen antagonist contraceptive hormone replacement therapy compn

# IT Mammary gland, neoplasm

Ovary, neoplasm

Prostate gland, neoplasm

Uterus, neoplasm

(carcinoma; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Selective estrogen receptor modulators

(codrugs; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Intestine, neoplasm

(colon, carcinoma; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Carcinoma

(colon; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Hemorrhage

(dysfunctional; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Carcinoma

(endometrial; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Uterus, disease

(endometriosis; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Uterus, neoplasm

(endometrium, carcinoma; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related

conditions)

IT Contraceptives

(female; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Uterus, neoplasm

(leiomyomata; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Carcinoma

(mammary; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Carcinoma

(ovarian; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Ovary, disease

(polycystic; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Carcinoma

(prostatic; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Antitumor agents

Carcinoma

Drug delivery systems

Hemostatics

Hormone replacement therapy

Human

(use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Antiandrogens

RL: BSU (Biological study, unclassified); BIOL (Biological study) (use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT Carcinoma

(uterine; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

304853-32-5P, 6-(3-Chlorophenyl)-4,4-dimethyl-1,4-IT dihydrobenzo[d][1,3]oxazin-2-thione 304853-33-6P, 4-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)thiophene-2-carbonitrile 304853-35-8P, 3-(4,4-Dimethyl-2-thioxo-1,4dihydro-2H-benzo[d][1,3]oxazin-6-yl)-5-fluorobenzonitrile 304853-37-0P, 3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2Hbenzo[d][1,3]oxazin-6-yl)benzonitrile 304853-38-1P, 6-(3-Fluorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-39-2P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1benzoxazin-6-yl)-4-methylthiophene-2-carbonitrile 304853-40-5P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-pyrrole-2carbonitrile 304853-41-6P, [6-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)pyridin-2-yl]acetonitrile 304853-42-7P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1Hpyrrole-2-carbonitrile 304853-43-8P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-pyrrole-2-carbothioamide 304853-44-9P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-

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benzo[d][1,3]oxazin-6-yl)thiophene-3-carbonitrile 304853-45-0P,
5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-ethyl-1H-
pyrrole-2-carbonitrile 304853-46-1P, 4-[1,2-Dihydro-2-
thioxospiro[4H-3,1-benzoxazin-4,1-cyclohexan]-6-yl]-2-
thiophenecarbonitrile 304853-47-2P, 5-(4,4-Dimethyl-2-thioxo-1,4-
dihydro-2H-3,1-benzoxazin-6-yl)-2-fluorobenzonitrile 304853-48-3P
  6-(5-Bromopyridin-3-yl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
thione 304853-49-4P, 6-(3-Chloro-5-fluorophenyl)-4,4-dimethyl-
1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-50-7P,
6-(3-Bromo-5-methylphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
thione 304853-51-8P, 6-(3-Bromo-5-trifluoromethoxyphenyl)-4,4-
dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-52-9P,
3-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1-cyclohexan]-6-yl]-5-
fluorobenzonitrile 304853-53-0P, 3-(4,4-Dimethyl-2-thioxo-1,4-
dihydro-2H-3,1-benzoxazin-6-yl)-5-methylbenzonitrile 304853-54-1P
  6-(3,5-Dichlorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
thione 304853-56-3P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
benzoxazin-6-yl)-2-furonitrile 304853-57-4P,
4,4-Diethyl-6-(3-nitrophenyl)-1,4-dihydro-2H-3,1-benzoxazine-2-thione
304853-58-5P, 6-(3-Chlorophenyl)-4-methyl-4-phenyl-1,4-dihydro-2H-
3,1-benzoxazine-2-thione 304853-59-6P, 4-Allyl-6-(3-
chlorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
304853-60-9P, 3-Chloro-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
benzoxazin-6-yl) benzonitrile 304853-61-0P, 6-(3,5-
Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
304853-62-1P, 6-(3-Fluoro-5-methoxyphenyl)-4,4-dimethyl-1,4-
dihydro-2H-3, 1-benzoxazine-2-thione 304853-63-2P,
3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-5-
methoxybenzonitrile 304853-64-3P, 6-(3-Fluorophenyl)-4,4-
dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-65-4P,
6-[3-Fluoro-5-(trifluoromethyl)phenyl]-4,4-dimethyl-1,4-dihydro-2H-3,1-
benzoxazine-2-thione 304853-66-5P, 6-(2-Fluorophenyl)-4,4-
dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-67-6P,
6-(3,4-Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
thione 304853-68-7P, 6-(4-Fluorophenyl)-4,4-dimethyl-1,4-dihydro-
2H-3,1-benzoxazine-2-thione 304853-69-8P, 3-(4,4-Dimethyl-2-
thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-4-fluorobenzonitrile
304853-70-1P, 6-(2,3-Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-
3,1-benzoxazine-2-thione 304853-71-2P, 3-(8-Bromo-4,4-dimethyl-2-
thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-5-fluorobenzonitrile
304853-72-3P, 4,4-Dimethyl-6-(3-nitrophenyl)-1,4-dihydro-2H-3,1-
benzoxazine-2-thione 304853-73-4P, 6-(3-Chlorophenyl)-4,4-
diethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-74-5P,
6-(3-Methoxyphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
304853-75-6P, 6-(2-Chlorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-
benzoxazine-2-thione 304853-76-7P, 4-Benzyl-6-(3-chlorophenyl)-4-
methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-77-8P,
6-(3-Bromo-5-fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
thione 304853-78-9P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
benzoxazin-6-yl)thiophene-2-carbonitrile 304853-79-0P,
3-Fluoro-5-(8-fluoro-4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-
yl)benzonitrile 304853-80-3P, 3-[1,2-Dihydro-2-thioxospiro[4H-
3,1-benzoxazine-4,1'-cyclohexan]-6-yl]benzonitrile 304853-81-4P,
5-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-4-
methyl-2-thiophenecarbonitrile 304853-82-5P,
5-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-2-
thiophenecarbonitrile 304853-83-6P, 6-(3-Chloro-4-fluorophenyl)-
4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-84-7P
, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-4-
propylthiophene-2-carbonitrile 304853-85-8P,
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4-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-2-furonitrile
304853-86-9P, 4-Butyl-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
benzoxazin-6-yl) thiophene-2-carbonitrile 304853-87-0P,
6-(3-Bromophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
304853-88-1P, 2-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
benzoxazin-6-yl)thiophene-3-carbonitrile 304853-95-0P,
2-Cyano-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-
pyrrole-1-carboxylic acid tert-Butyl ester 638989-33-0P,
1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclobutan]-6-
yl]-1H-pyrrole-2-carbonitrile 638989-38-5P, 5-(4,4-Diethyl-2-
thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-
carbonitrile 638989-41-0P, 5-(4-Ethyl-4-methyl-2-thioxo-1,4-
dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile
638989-44-3P, 1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-
benzoxazine-4,1'-cyclohexan]-6-yl]-1H-pyrrole-2-carbonitrile
638989-46-5P, 1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-
benzoxazine-4,1'-cyclopentan]-6-yl]-1H-pyrrole-2-carbonitrile
638989-48-7P, 1-Methyl-5-[2-thioxo-4,4-bis(trifluoromethyl)-1,4-
dihydro-2H-3,1-benzoxazin-6-yl]-1H-pyrrole-2-carbonitrile
639085-00-0P, 5-(4,4-Dimethyl-1,2-thioxo-1,4-dihydro-2H-3,1-
benzoxazin-6-yl)isophthalonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; use of cyclothiocarbamate derivs. as selective
   androgen antagonists in contraception, hormone replacement therapy and
   in treatment of other hormone-related conditions)
50-41-9, Clomiphene citrate
                              1845-11-0, Nafoxidene
                                                      31477-60-8,
Centchroman
             54965-24-1, Tamoxifen citrate
                                              78994-23-7, Levormeloxifene
82413-20-5, Droloxifene 82640-04-8, Raloxifene hydrochloride
89778-27-8, Toremifene citrate
                                 116057-75-1, Idoxifene
                                                          180916-16-9,
Lasofoxifene
               182133-25-1, Arzoxifene
                                        182167-02-8, EM-652
182167-03-9, EM-800
                      198480-55-6, Pipendoxifene
                                                   198481-32-2,
               638186-49-9
Bazedoxifene
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
   (selective estrogen receptor modulator as codrug; use of
   cyclothiocarbamate derivs. as selective androgen antagonists in
   contraception, hormone replacement therapy and in treatment of other
   hormone-related conditions)
684-16-2, Hexafluoroacetone
                              1191-95-3, Cyclobutanone
                                                         3422-01-3
29124-56-9, 1-(2-Amino-5-bromophenyl)ethanone
                                                34884-10-1,
1-Methyl-1H-pyrrole-2-carbonitrile 304854-04-4,
6-Bromospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one
305799-84-2, 6-Bromospiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2-
(1H) -one 638989-40-9, 6-Bromo-4,4-diethyl-1,4-
dihydrobenzo[d][1,3]oxazin-2-one
RL: RCT (Reactant); RACT (Reactant or reagent)
   (use of cyclothiocarbamate derivs. as selective androgen antagonists in
   contraception, hormone replacement therapy and in treatment of other
   hormone-related conditions)
2713-62-4P, 2-(2-Aminophenyl)-1,1,1,3,3,3-hexafluoropropan-2-ol
638989-34-1P, tert-Butyl [2-(1-hydroxycyclobutyl)phenyl]carbamate
638989-35-2P, Spiro[3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one
638989-36-3P, 6-Bromospiro[3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-
one 638989-37-4P, 1-Methyl-5-[2-oxo-1,2-dihydrospiro[3,1-
benzoxazine-4,1'-cyclobutan]-6-yl]-1H-pyrrole-2-carbonitrile
638989-39-6P, 5-(4,4-Diethyl-2-oxo-1,4-dihydro-2H-3,1-benzoxazin-6-
yl)-1-methyl-1H-pyrrole-2-carbonitrile 638989-42-1P,
6-Bromo-4-ethyl-4-methyl-1,4-dihydro-2H-3,1-benzoxazin-2-one
638989-43-2P, 5-(4-Ethyl-4-methyl-2-oxo-1,4-dihydro-2H-3,1-
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ΙT

TT

IT

benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile 638989-45-4P
, 1-Methyl-5-[2-oxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclohexan]-6yl]-1H-pyrrole-2-carbonitrile 638989-47-6P, 1-Methyl-5-[2-oxo1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclopentan]-6-yl]-1H-pyrrole-2carbonitrile 638989-49-8P, 4,4-Bis(trifluoromethyl)-1,4-dihydro2H-3,1-benzoxazin-2-one 638989-50-1P, 6-Bromo-4,4bis(trifluoromethyl)-1,4-dihydro-2H-3,1-benzoxazin-2-one
638989-51-2P, 1-Methyl-5-[2-oxo-4,4-bis(trifluoromethyl)-1,4dihydro-2H-3,1-benzoxazin-6-yl]-1H-pyrrole-2-carbonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

IT 304853-32-5P, 6-(3-Chlorophenyl)-4,4-dimethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-thione

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; use of cyclothiocarbamate derivs. as selective androgen antagonists in contraception, hormone replacement therapy and in treatment of other hormone-related conditions)

RN 304853-32-5 HCAPLUS

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

L119 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:2636 HCAPLUS

DN 140:53469

ED Entered STN: 02 Jan 2004

TI Cyclothiocarbamate derivatives as progesterone receptor modulators and use thereof for treatment of skin disorders

IN Fensome, Andrew; Harrison, Diane Deborah; Winneker, Richard Craig; Zhang, Puwen; Kern, Jeffrey Curtis; Terefenko, Eugene Anthony

PA Wyeth, John, and Brother Ltd., USA

SO PCT Int. Appl., 83 pp. CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K

CC 1-12 (Pharmacology)

Section cross-reference(s): 27

FAN.CNT 1

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PI	WO	200	40002	30		A2		2003	1231	1	WO 2	003-1	US19	860	60 200306				523 <
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GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
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CLASS
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                       PATENT FAMILY CLASSIFICATION CODES
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                       WO 2004000230
                ICM
                       A61K
 WO 2004000230
                ECLA
                        A61K008/49; A61K031/536; A61K031/536+M; A61K031/565+M;
                       A61Q007/00; A61Q019/00
US 2004014798
                NCL
                        514/369.000
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     MARPAT 140:53469
AΒ
     The present invention provides for the use of a compds. that
     modulate progesterone receptors and thereby
     treat skin disorders. Specifically, methods for treating acne,
     hirsutism, and conditioning the skin are described.
ST
     progesterone receptor modulator
     cyclothiocarbamate deriv skin disease
IT
     Eczema
      Hirsutism
       Skin, disease
        (cyclothiocarbamate derivs. as progesterone receptor
       modulators and use thereof for treatment of skin disorders)
IT
     Antiandrogens
       Antiprogestins
       Progesterone receptors
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (cyclothiocarbamate derivs. as progesterone receptor
       modulators and use thereof for treatment of skin disorders)
     Drug delivery systems
IT
        (injections; cyclothiocarbamate derivs. as progesterone
        receptor modulators and use thereof for treatment of
        skin disorders)
IT
     Drug delivery systems
        (tablets; cyclothiocarbamate derivs. as progesterone
        receptor modulators and use thereof for treatment of
        skin disorders)
IT
     Acne
        (vulgaris; cyclothiocarbamate derivs. as progesterone
        receptor modulators and use thereof for treatment of
        skin disorders)
IT
     638989-33-0P 638989-38-5P 638989-41-0P
     638989-44-3P 638989-46-5P 638989-48-7P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (cyclothiocarbamate derivs. as progesterone receptor
       modulators and use thereof for treatment of skin disorders)
IT
     304853-32-5 304853-35-8 304853-37-0
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304853-38-1 304853-39-2 304853-40-5
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     304853-44-9 304853-45-0 304853-46-1
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     304853-50-7 304853-51-8 304853-52-9
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     304853-69-8 304853-70-1 304853-71-2
     304853-72-3 304853-73-4 304853-74-5
     304853-75-6 304853-76-7 304853-77-8
     304853-78-9 304853-79-0 304853-80-3
     304853-81-4 304853-82-5 304853-83-6
     304853-84-7 304853-85-8 304853-86-9
     304853-87-0 304853-88-1 304853-95-0
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (cyclothiocarbamate derivs. as progesterone receptor
        modulators and use thereof for treatment of skin disorders)
IT
     684-16-2, Hexafluoroacetone
                                  1191-95-3, Cyclobutanone
     29124-56-9
                  34884-10-1, 1-Methyl-1H-pyrrole-2-carbonitrile
     304854-04-4 305799-84-2 638989-40-9
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclothiocarbamate derivs. as progesterone receptor
        modulators and use thereof for treatment of skin disorders)
IT
     2713-62-4P 638989-34-1P 638989-35-2P 638989-36-3P
     638989-37-4P 638989-39-6P 638989-42-1P
     638989-43-2P 638989-45-4P 638989-47-6P
     638989-49-8P 638989-50-1P 638989-51-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (cyclothiocarbamate derivs. as progesterone receptor
        modulators and use thereof for treatment of skin disorders)
IT
     57-83-0, Progesterone, biological studies
                                                 797-63-7,
     Levonorgestrel 54048-10-1, 3-Ketodesogestrel
     RL: PAC (Pharmacological activity); BIOL (Biological study)
        (reference compound; cyclothiocarbamate derivs. as progesterone
        receptor modulators and use thereof for treatment of
        skin disorders)
IT
     638989-33-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (cyclothiocarbamate derivs. as progesterone receptor
        modulators and use thereof for treatment of skin disorders)
     638989-33-0 HCAPLUS
RN
     1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-
CN
     4,1'-cyclobutan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)
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L119 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN
     2002:669675 HCAPLUS
AN
DN
     137:201317
ED
     Entered STN: 05 Sep 2002
     Preparation of benzoxazinone cyclic carbamate antiprogestins for use in
TI
     combination therapies and regimens with progestational agents.
IN
     Grubb, Gary S.; Zhang, Puwen; Terefenko, Eugene A.;
     Fensome, Andrew; Wrobel, Jay E.; Fletcher, Iii Horace; Edwards,
     James P.; Jones, Todd K.; Tegley, Christopher M.; Zhi, Lin
PA
     Wyeth, John and Brother Ltd., USA; Ligand Pharmaceuticals
     Incorporated
SO
     U.S., 44 pp.
     CODEN: USXXAM
DT
     Patent
     English
LA
IC
     ICM A61K031-535
     ICS A61K031-56
INCL 514230500
     28-13 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1, 2
FAN.CNT 3
     PATENT NO.
                                            APPLICATION NO.
                         KIND
                                DATE
                                                                    DATE
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                                            US 2000-552350
PΙ
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                         Т3
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                          Α
                                20000419
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     WO 2000-US11643
                          W
                                20000501
CLASS
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US 6444668
                 ICM
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                 ICS
                        A61K031-56
                 INCL
                        514230500
US 6444668
                 NCL
                        514/230.500; 514/178.000; 514/843.000
                 ECLA
                        A61K031/535+M; A61K031/56+M
US 2003045511
                 NCL
                        514/230.500; 514/170.000; 514/171.000; 514/178.000;
                        514/182.000; 514/228.800; 514/230.800; 514/247.000;
                        514/359.000; 514/843.000
                 ECLA
                        A61K031/535+M; A61K031/56+M
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os
    MARPAT 137:201317
GI
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A method of contraception comprises administration to a female of a AB progestational agent in a first phase and in a second phase administration of [I; R1, R2 = H, (un) substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, aryl, heterocyclyl, amino derivative; R1R2 = atoms to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, C3-6 alkenyl, alkynyl, COR6; R6 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, CN, NO2, (un) substituted C1-6 alkyl, alkynyl, C1-6 alkoxy, amino, C1-6 aminoalkyl; R5 = trisubstituted benzene ring, 5-6 membered ring with 1, 2, or 3 O, S, SO, SO2, NR7 and containing 1-2 H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, NR9COR8; R7 = H, C1-3 alkyl; R8 = H, (un) substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R9 = H, (un) substituted C1-3 alkyl]. Thus, 6-(3-chlorophenyl)-4,4-dimethyl-1,4dihydrobenzo[d][1,3]-oxazin-2-one was prepared from 2-(2-amino-5bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. I demonstrated IC50's of 2.7-68 nM in a hPR decidualization assay. ST cyclocarbamate aryl prepn antiprogestin combination therapy regimen progestational agent; benzoxazinone prepn progesterone receptor antagonist; oxazinone benzo prepn progesterone receptor antagonist; contraceptive benzoxazinone antiprogestin progestin IT Contraceptives

(preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

IT Progesterone receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study) (preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

IT Antiprogestins

Human

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

IT Estrus

(regulation of; preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

IT 51-98-9, Norethindrone acetate 68-22-4, Norethindrone 427-51-0, 797-63-7, Levonorgestrel Cyproterone acetate 6533-00-2, Norgestrel 35189-28-7, Norgestimate 53016-31-2, 17-Deacetylnorgestimate 54048-10-1, 3-KetoDesogestrel 54024-22-5, Desogestrel 58691-88-6, Nomegestrol 60282-87-3, Gestodene 65928-58-7, Dienogest 67392-87-4, 74513-62-5, Trimegestone 105149-04-0, Osaterone Drospirenone RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (combination therapy; preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

IT 304853-93-8P, 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-dihydro-4-304853-94-9P, 2-Thiophenecarbonitrile, 5-(1,4-dihydro-4,4dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-methyl-304853-98-3P, 2-Pyridineacetonitrile, 6-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1benzoxazin-6-yl)-304854-01-1P, 3-Thiophenecarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents) ΙT 304853-28-9P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4,4-304853-29-0P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5fluorophenyl) -1, 4-dihydro-4, 4-dimethyl-304853-30-3P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro-304853-31-4P, 2-Thiophenecarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-304853-36-9P, Benzonitrile, 2H-3,1-benzoxazin-6-yl)-3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-304853-96-1P, 1H-Pyrrole-1-carboxylic acid, 2-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1benzoxazin-6-yl)-, 1,1-dimethylethyl ester 304854-06-6P, 2-Thiophenecarbonitrile, 4-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'cyclohexan]-6-yl)- 304854-07-7P, Benzonitrile, 5-(1,4-dihydro-4,4dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro-304854-08-8P, 2H-3,1-Benzoxazin-2-one, 6-(5-bromo-3-pyridinyl)-1,4-dihydro-4,4-dimethyl-304854-09-9P, 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-5-fluorophenyl)-1,4dihydro-4,4-dimethyl- 304854-10-2P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-methylphenyl)-1,4-dihydro-4,4-dimethyl-304854-11-3P, 2H-3,1-Benzoxazin-2-one, 6-[3-bromo-5-(trifluoromethoxy)phenyl]-1,4-304854-12-4P, Benzonitrile, 3-(1,2-dihydro-2dihydro-4,4-dimethyloxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-5-fluoro-304854-13-5P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-304854-14-6P, 2H-3,1-Benzoxazin-2-one, benzoxazin-6-yl)-5-methyl-6-(3,5-dichlorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-15-7P, 1,3-Benzenedicarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1benzoxazin-6-yl) - 304854-16-8P, 2-Furancarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-304854-17-9P, 2H-3,1-Benzoxazin-2-one, 4,4-diethyl-1,4-dihydro-6-(3-nitrophenyl)-304854-20-4P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-304854-21-5P, 2H-3,1-Benzoxazin-2-one, methyl-4-phenyl-6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(2-propenyl)-304854-22-6P, Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-304854-23-7P, 2H-3,1-Benzoxazin-2-one, 6-(3,5-difluorophenyl)-1,4-6-yl)-304854-24-8P, 2H-3,1-Benzoxazin-2-one, dihydro-4,4-dimethyl-6-(3-fluoro-5-methoxyphenyl)-1,4-dihydro-4,4-dimethyl-304854-25-9P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-304854-26-0P, 2H-3,1-Benzoxazin-2-one, 6-(3-fluorophenyl)-1,4-304854-27-1P, 2H-3,1-Benzoxazin-2-one, dihydro-4,4-dimethyl-6-[3-fluoro-5-(trifluoromethyl)phenyl]-1,4-dihydro-4,4-dimethyl-304854-28-2P, 2H-3,1-Benzoxazin-2-one, 6-(2-fluorophenyl)-1,4-dihydro-4,4-304854-29-3P, 2H-3,1-Benzoxazin-2-one, 6-(3,4-difluorophenyl)dimethyl-304854-30-6P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-dimethyl-6-(4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- 304854-31-7P, Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro-304854-32-8P, 2H-3,1-Benzoxazin-2-one, 6-(2,3-difluorophenyl)-1,4-dihydro-304854-33-9P, Benzonitrile, 3-(8-bromo-1,4-dihydro-4,4-4,4-dimethyldimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro-304854-34-0P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-dimethyl-6-(3-nitrophenyl)-304854-35-1P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4,4-diethyl-1,4-304854-36-2P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-6-(3-

methoxyphenyl)-4,4-dimethyl-

304854-37-3P, 2H-3,1-Benzoxazin-2-one,

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6-(2-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
                                             304854-38-4P,
2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-
                304854-39-5P, 2-Thiophenecarbonitrile,
(phenylmethyl) -
5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
                                                             304854-41-9P,
Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-
                   304854-42-0P, Benzonitrile, 3-(1,2-dihydro-2-
benzoxazin-6-yl)-
oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-
                                                     304854-43-1P,
2-Thiophenecarbonitrile, 5-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-
cyclohexan]-6-yl)-4-methyl-
                             304854-44-2P, 2-Thiophenecarbonitrile,
5-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-
304854-45-3P, 2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-1,4-
dihydro-4,4-dimethyl-
                        304854-46-4P, 2-Thiophenecarbonitrile,
5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-propyl-
304854-47-5P, 2-Furancarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-
3,1-benzoxazin-6-yl)-
                       304854-48-6P, 2-Thiophenecarbonitrile,
4-butyl-5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
304854-49-7P, 2H-3,1-Benzoxazin-2-one, 6-(3-bromophenyl)-1,4-dihydro-4,4-
           304854-50-0P, 3-Thiophenecarbonitrile, 2-(1,4-dihydro-4,4-
dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
                                          305799-74-0P,
2H-3,1-Benzoxazin-2-one, 6-(4-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
305799-76-2P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-1,4-dihydro-4-
          305799-78-4P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-
ethyl-1,4-dihydro-
                    305799-80-8P, 2H-3,1-Benzoxazin-2-one,
6-(3-chlorophenyl)-1,4-dihydro-4-phenyl-
                                           305799-81-9P,
3-Pyridinecarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-
benzoxazin-6-yl)-
                   305799-83-1P, Spiro[4H-3,1-benzoxazine-4,1'-
cyclohexan] -2-one, 6-(3-chlorophenyl) -1,2-dihydro-
                                                    305799-85-3P,
Spiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-one, 6-(3-chlorophenyl)-
305799-86-4P, Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2-one,
1,2-dihydro-6-(3-nitrophenyl)- 305799-87-5P, 2H-3,1-Benzoxazin-2-one,
6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(1-propynyl)-
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2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-ethynyl-1,4-dihydro-4-methyl-
   305799-89-7P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4-cyclopropyl-
1,4-dihydro-4-methyl-
                       305799-93-3P, 2H-3,1-Benzoxazin-2-one,
6-(3-chlorophenyl)-4-cyclopropyl-1,4-dihydro-4-(1-propynyl)-
305799-95-5P, 2H-3,1-Benzoxazin-2-one, 6-(3-chlorophenyl)-4,4-
                            305799-97-7P, 2H-3,1-Benzoxazin-2-one,
dicyclopropyl-1,4-dihydro-
6-(3-chlorophenyl)-1,4-dihydro-4,4-di-1-propynyl-
                                                   305799-98-8P,
2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-1,4,4-
             305799-99-9P, 2H-3,1-Benzoxazin-2-one, 6-chloro-1,4-dihydro-4-
trimethyl-
methyl-4-(trifluoromethyl)- 305800-00-4P, 2H-3,1-Benzoxazin-2-one,
1,4-dihydro-6-(3-methoxyphenyl)-4-methyl-4-(trifluoromethyl)-
305800-02-6P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-7-(3-methoxyphenyl)-4,4-
dimethyl-
           305800-03-7P, 2H-3,1-Benzoxazin-2-one, 6-(3-acetylphenyl)-1,4-
dihydro-4,4-dimethyl-
                      305800-04-8P, 2H-3,1-Benzoxazin-2-one,
6-(3-benzoylphenyl)-1,4-dihydro-4,4-dimethyl-
                                                305800-05-9P,
2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-dimethyl-6-[3-(1H-tetrazol-5-
             305800-08-2P, 2-Thiophenecarbonitrile, 4-(4,4-dicyclopropyl-
yl)phenyl]-
1,4-dihydro-2-oxo-2H-3,1-benzoxazin-6-yl)-
                                             305800-09-3P,
2H-3,1-Benzoxazin-2-one, 6-(3-bromo-5-fluorophenyl)-4,4-dicyclopropyl-1,4-
dihydro-
           305800-10-6P, Benzonitrile, 3-(4,4-dicyclopropyl-1,4-dihydro-2-
oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro-
                                      305800-11-7P, Benzonitrile,
3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-
(trifluoromethoxy) -
                     305800-12-8P, 2H-3,1-Benzoxazin-2-one,
6-[3,5-bis(trifluoromethyl)phenyl]-1,4-dihydro-4,4-dimethyl-
305800-14-0P, Benzonitrile, 3-[1-(diethoxymethyl)-1,4-dihydro-4,4-dimethyl-
2-oxo-2H-3,1-benzoxazin-6-yl]-5-fluoro-
                                         305800-15-1P, Benzonitrile,
3-[1,4-dihydro-1-(methoxymethyl)-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-
              305800-16-2P, Phosphoric acid, 6-(3-cyano-5-fluorophenyl)-
yl]-5-fluoro-
4,4-dimethyl-4H-3,1-benzoxazin-2-yl diethyl ester 305800-18-4P,
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2H-3,1-Benzoxazin-2-one, 6-(3-chloro-4-fluorophenyl)-8-fluoro-1,4-dihydro-
4,4-dimethyl-
               305800-19-5P, 2H-3,1-Benzoxazin-2-one,
1,4-dihydro-4,4-dimethyl-6-[3-[(trimethylsilyl)ethynyl]phenyl]-
305800-20-8P, 2H-3,1-Benzoxazin-2-one, 6-(3-ethynylphenyl)-1,4-dihydro-4,4-
           305800-21-9P, 2-Propynenitrile, 3-[3-(1,4-dihydro-4,4-dimethyl-
2-oxo-2H-3,1-benzoxazin-6-yl)phenyl]- 305800-22-0P, 2H-3,1-Benzoxazin-2-
one, 6-(3-fluoro-5-nitrophenyl)-1,4-dihydro-4,4-dimethyl-
                                                           305800-23-1P,
2H-3,1-Benzoxazin-2-one, 6-(3,5-dinitrophenyl)-1,4-dihydro-4,4-dimethyl-
305800-24-2P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-dimethyl-6-[3-(2-
thiazolyl)phenyl]-
                    305800-25-3P, 2H-3,1-Benzoxazin-2-one,
6-(5-bromo-1-oxido-3-pyridinyl)-1,4-dihydro-4,4-dimethyl-
                                                            305800-26-4P,
2H-3,1-Benzoxazine-1(4H)-carboxylic acid, 6-(3-cyano-5-fluorophenyl)-4,4-
dimethyl-2-oxo-, 1,1-dimethylethyl ester
                                          305800-27-5P,
2-Thiophenecarbonitrile, 4-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-
                   305800-34-4P, 2H-3,1-Benzoxazin-2-one,
benzoxazin-6-yl)-
1,4-dihydro-4,4-dimethyl-6-[3-(1,2,4-thiadiazol-3-yl)phenyl]-
305800-36-6P, 1H-Pyrrole-1-carboxylic acid, 2-(1,4-dihydro-4,4-dimethyl-2-
oxo-2H-3,1-benzoxazin-6-yl)-5-nitro-,1,1-dimethylethylester
305800-37-7P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-dimethyl-6-(5-nitro-
                 305800-38-8P, 2H-3,1-Benzoxazin-2-one,
1H-pyrrol-2-yl)-
1,4-dihydro-4,4-dimethyl-6-(1H-pyrrol-2-yl)-
                                              305800-39-9P,
2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-dimethyl-6-(1-methyl-1H-pyrrol-2-
       305800-40-2P, 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-dimethyl-6-
                                   305800-45-7P, 2-
(1-methyl-5-nitro-1H-pyrrol-2-yl)-
Thiophenecarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-
               305800-46-8P, Benzonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-
6-yl)-4-ethyl-
oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro-
                                      305800-47-9P, Benzeneacetonitrile,
3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
                                                             305800-48-0P,
Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-
fluoro-
         305800-50-4P, Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-
one, 6-(3-methoxyphenyl)-
                           305800-51-5P, 2H-3,1-Benzoxazin-2-one,
8-bromo-6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl-
305800-52-6P, Benzonitrile, 5-(8-bromo-1,4-dihydro-4,4-dimethyl-2-oxo-2H-
3,1-benzoxazin-6-yl)-2-fluoro- 305800-53-7P, 2H-3,1-Benzoxazin-2-one,
6-(3-bromophenyl)-1,4-dihydro-1,4,4-trimethyl-
                                                 305800-55-9P,
Benzonitrile, 3-(1,4-dihydro-8-methoxy-4,4-dimethyl-2-oxo-2H-3,1-
benzoxazin-6-yl)-5-fluoro- 305800-56-0P, Benzonitrile,
3-(1,4-dihydro-8-hydroxy-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-5-
         305800-57-1P, Benzonitrile, 3-(1-ethyl-1,4-dihydro-4,4-dimethyl-
2-oxo-2H-3,1-benzoxazin-6-yl)-5-fluoro-
                                        305800-59-3P,
Benzeneacetonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-
               305800-62-8P, Benzeneacetonitrile, 4-(1,4-dihydro-4,4-
yl)-5-fluoro-
dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-2-fluoro- 305800-63-9P,
Benzeneacetonitrile, 2-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-
       305800-64-0P, Acetamide, N-[4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-
3,1-benzoxazin-6-yl)-2-fluorophenyl]- 305800-65-1P, 2H-3,1-Benzoxazin-2-
one, 6-(3-fluoro-4-methoxyphenyl)-1,4-dihydro-4,4-dimethyl-
305800-66-2P, Benzenesulfonamide, 3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-
benzoxazin-6-yl) - 305800-67-3P, 2-Thiophenesulfonamide,
5-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
                                                             305800-68-4P,
2H-3,1-Benzoxazin-2-one, 6-(6-amino-3-pyridinyl)-1,4-dihydro-4,4-dimethyl-
305800-71-9P, 2-Furancarboxaldehyde, 4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-
3,1-benzoxazin-6-yl) - 305800-72-0P, 2-Furancarboxaldehyde,
4-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-, 2-oxime
305839-71-8P, 2H-3,1-Benzoxazin-2-one, 6-[3-fluoro-5-(2-thienyl)phenyl]-
1,4-dihydro-4,4-dimethyl- 305839-75-2P, Benzeneacetonitrile,
3-(1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-4-fluoro-
305839-76-3P, 2H-3,1-Benzoxazin-2-one, 6-[5-(diethoxymethyl)-2-furanyl]-
1,4-dihydro-4,4-dimethyl-
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
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(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents) ΙT 100-58-3, Phenylmagnesium bromide 108-36-1, 1,3-Dibromobenzene 110-52-1, 1,4-Dibromobutane 111-24-0, 1,5-Dibromopentane Triethylorthoformate 326-66-9, 4'-Bromo-2'-fluoroacetanilide 348-61-8, 1-Bromo-3,4-difluorobenzene 460-00-4, 1-Bromo-4-fluorobenzene 461-96-1, 1-Bromo-3,5-difluorobenzene 623-49-4, Ethylcyano formate 625-92-3, 3,5-Dibromopyridine 814-49-3, Diethyl chlorophosphate 1066-54-2, Trimethylsilylacetylene 1072-85-1, 1-Bromo-2-fluorobenzene 1072-97-5, 2-Amino-5-bromopyridine 1073-06-9, 1-Bromo-3-fluorobenzene 1191-95-3, Cyclobutanone 1435-51-4, 1,3-Dibromo-5-fluorobenzene 1546-79-8, 1-(Trifluoroacetyl)imidazole 1611-92-3, 3,5-Dibromotoluene 1679-18-1, 4-Chlorophenyl boronic acid 1730-25-2, Allylmagnesium bromide 2357-52-0, 4-Bromo-2-fluoroanisole 3177-80-8, 2-Amino-3-methoxybenzoic 3900-89-8, 2-Chlorophenyl boronic acid 4333-56-6, Cyclopropyl bromide 4648-54-8, Trimethylsilyl azide 4692-98-2, 5-Bromoisatoic anhydride 4701-17-1, 5-Bromo-2-thiophenecarboxaldehyde 4915-06-4, 2-Bromo-5-cyanofuran 5326-47-6, 2-Amino-5-iodobenzoic acid 5794-88-7. 6165-69-1, 3-Thiophene boronic acid 2-Amino-5-bromobenzoic acid 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6952-59-6, 3-Bromobenzonitrile 7087-65-2, Benzene, 1-bromo-3-fluoro-5-nitro-10365-98-7, 3-Methoxyphenyl boronic acid 13331-27-6, 3-Nitrophenyl boronic acid 14282-76-9, 2-Bromo-3-methylthiophene 18242-39-2, 1-Bromo-3,5-dinitrobenzene 18791-99-6, 2-Thiophenecarbonitrile, 4-bromo-18792-00-2, 3-Thiophenecarbonitrile, 5-bromo- 19472-74-3, 2-Bromophenylacetonitrile 27065-51-6, Furan, 4-bromo-2-(diethoxymethyl)-29578-39-0, Anisole, 3-Bromo-5-fluoro-31938-07-5, 3-32423-84-0, Propynylmagnesium bromide Bromophenylacetonitrile 33743-87-2, 1,3,4-Oxathiazol-2-one, 5-(3-bromophenyl)-33863-76-2, 35590-37-5, 3-Bromo-5-cyanopyridine 1-Bromo-3-chloro-5-fluorobenzene 39263-32-6, 2-Amino-5-bromobenzonitrile 51437-00-4, 5-Bromo-2-53119-61-2, 2-Bromo-3-ethylthiophene fluorotoluene 53595-65-6, 2-Thiophenesulfonamide, 5-bromo-56182-43-5, 2-Bromo-3thiophenecarbonitrile 60811-21-4, Benzene, 4-bromo-2-chloro-1-fluoro-63503-60-6, 3-Chlorophenyl boronic acid 65854-91-3, N-(4-Chlorophenyl)-2,2-dimethylpropanamide 67492-50-6, 3,5-Dichlorophenyl boronic acid 69249-60-1, Thiophene, 2-bromo-3-propyl- 73852-19-4, Boronic acid, [3,5-bis(trifluoromethyl)phenyl]-89599-01-9, 3-Bromobenzenesulfonamide 112575-11-8, 105942-08-3, Benzonitrile, 4-bromo-2-fluoro-2-Pyridineacetonitrile, 6-bromo- 114897-91-5, Benzeneacetonitrile, 121359-48-6, Thiazole, 2-(tributylstannyl)-4-bromo-2-fluoro-130723-13-6, Benzene, 1-bromo-3-fluoro-5-(trifluoromethyl)-1H-Pyrrole-1-carboxylic acid, 2-borono-, 1-(1,1-dimethylethyl) ester 145543-82-4, 2-Bromo-3-n-butylthiophene 160892-07-9, 5-Bromoisophthalonitrile 161957-56-8, Benzoic acid, 3-bromo-2-fluoro-179897-89-3, Benzonitrile, 5-bromo-2-fluoro-179898-34-1, 3-Bromo-5-fluorobenzonitrile 188813-02-7, Benzaldehyde, 207226-31-1, Benzene, 1,3-dibromo-5-(trifluoromethoxy)-3-bromo-5-fluoro-216755-57-6, Benzene, 1-bromo-3-(bromomethyl)-5-fluoro-304854-51-1, [1,1'-Biphenyl]-3-carbonitrile, 4-amino-3'-fluoro-304854-53-3, 2H-3,1-Benzoxazin-2-one, 4,4-diethyl-1,4-dihydro-6-iodo-304854-55-5, 304854-57-7, Methanesulfonic acid, Benzonitrile, 3-bromo-5-chlorotrifluoro-, (2,3-difluorophenyl) methyl ester 304854-59-9, [1,1'-Biphenyl]-3-methanol, 4-amino-3'-chloro- $\alpha$ -methyl- $\alpha$ -304854-61-3, Boronic acid, (8-fluoro-1,4-dihydro-4,4-(phenylmethyl) dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-304854-63-5, 2-Furancarbonitrile, 4-bromo-305799-77-3, [1,1'-Biphenyl]-3-methanol, 4-amino-3'-chloro- $\alpha$ -ethyl- 305799-79-5, [1,1'-Biphenyl]-3-

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methanol, 4-amino-3'-chloro-α-phenyl-
                                            305799-92-2,
     [1,1'-Biphenyl]-3-methanol, 4-amino-3'-chloro-\alpha-cyclopropyl-\alpha-
                   305800-01-5, 2H-3,1-Benzoxazin-2-one, 7-chloro-1,4-dihydro-
     1-propynyl-
     4,4-dimethyl-
                     305800-13-9, Methanesulfonic acid, trifluoro-,
     3-cyano-5-methoxyphenyl ester
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of benzoxazinone cyclic carbamate antiprogestins for use in
        combination therapies and regimens with progestational agents)
IT
     2160-62-5P, 2-Thiophenecarbonitrile, 5-bromo-
                                                      21440-97-1P,
     2H-3,1-Benzoxazin-2-one, 6-bromo-1,4-dihydro-4,4-dimethyl-
                                                                   21440-99-3P,
     2H-3,1-Benzoxazin-2-one, 1,4-dihydro-8-methoxy-4,4-dimethyl-
     141940-30-9P, Benzoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-
               149947-15-9P, Benzaldehyde, 3-bromo-2-fluoro-
                                                                154598-53-5P,
     Ethanone, 1-(2-amino-5-chlorophenyl)-2,2,2-trifluoro-
                                                              189331-47-3P,
     2-Thiophenecarboxaldehyde, 5-bromo-4-methyl-
                                                    206551-41-9P, Benzoic acid,
     3-bromo-2-fluoro-, methyl ester
                                      216755-56-5P, Benzenemethanol,
     3-bromo-5-fluoro-
                         304853-89-2P, Benzenemethanol, 2-amino-5-bromo-
     \alpha, \alpha-dimethyl-
                     304853-90-5P, Boronic acid,
     (1,4-dihydro-4,4-dimethyl-2-oxo-2H-3,1-benzoxazin-6-yl)-
                                                                 304853-91-6P,
     Ethanone, 1-(4-amino-3'-fluoro[1,1'-biphenyl]-3-yl)-
                                                           304853-92-7P,
     [1,1'-Biphenyl]-3-methanol, 4-amino-3'-fluoro-\alpha-methyl-
     304854-03-3P, Cyclohexanol, 1-(2-amino-5-bromophenyl)-
     304854-04-4P, Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2-one,
     6-bromo-1,2-dihydro-
                            304854-05-5P, Boronic acid, (1,2-dihydro-2-
     oxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-
                                                            304854-19-1P,
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                                                             304854-40-8P,
     2H-3,1-Benzoxazin-2-one, 8-fluoro-1,4-dihydro-4,4-dimethyl-
     304854-52-2P, 2-Thiophenecarbonitrile, 5-bromo-4-methyl-
                                                                 304854-54-4P,
     Benzamide, 2-amino-5-bromo-N-methoxy-N-methyl-
                                                      304854-58-8P,
     2H-3,1-Benzoxazin-2-one, 1,4-dihydro-6-iodo-4,4-dimethyl-
                                                                  304854-62-4P,
     2-Thiophenecarbonitrile, 5-bromo-4-propyl-
                                                   304857-58-7P,
     [1,1'-Biphenyl]-3-carbonitrile, 4-amino-3'-chloro-
                                                           304874-29-1P,
     2-Thiophenecarbonitrile, 5-bromo-4-butyl-
                                                 305799-75-1P.
     [1,1'-Biphenyl]-3-methanol, 4-amino-3'-chloro-\alpha-methyl-
     305799-84-2P, Spiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-
     one, 6-bromo- 305799-94-4P, [1,1'-Biphenyl]-3-methanol,
     4-amino-3'-chloro-\alpha, \alpha-dicyclopropyl-
                                            305799-96-6P,
     2-Butyn-1-one, 1-(4-amino-3'-chloro[1,1'-biphenyl]-3-yl)-
                                                                  305800-06-0P,
     Boronic acid, (4,4-dicyclopropyl-1,4-dihydro-2-oxo-2H-3,1-benzoxazin-6-yl)-
        305800-17-3P, 2H-3,1-Benzoxazin-2-one, 6-bromo-8-fluoro-1,4-dihydro-4,4-
                 305800-29-7P, 1,2,4-Thiadiazole-5-carboxylic acid,
     3-(3-bromophenyl)-, ethyl ester
                                      305800-32-2P, 1,2,4-Thiadiazole,
     3-(3-bromophenyl)-
                          305800-41-3P, 2-Thiophenecarboxaldehyde,
                        305800-42-4P, 2-Thiophenecarbonitrile, 5-bromo-4-ethyl-
     5-bromo-4-ethyl-
     305800-43-5P, 2-Thiophenecarboxaldehyde, 5-bromo-4-propyl-
                                                                   305800-44-6P,
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     2-Thiophenecarboxaldehyde, 5-bromo-4-butyl-
     Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one, 6-chloro-
     305800-54-8P, 2H-3,1-Benzoxazin-2-one, 6-bromo-1,4-dihydro-8-methoxy-4,4-
                 305839-72-9P, [1,1'-Biphenyl]-3-carboxamide,
     dimethyl-
     3'-chloro-N-methoxy-N-methyl-
                                    305839-73-0P, Methanone,
     (4-amino-3'-chloro[1,1'-biphenyl]-3-yl)cyclopropyl-, hydrochloride
     305839-74-1P, [1,1'-Biphenyl]-3-methanol, 4-amino-3'-chloro-\alpha-
     cyclopropyl-
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of benzoxazinone cyclic carbamate antiprogestins for use in
        combination therapies and regimens with progestational agents)
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- IT 304854-04-4P, Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2-one, 6-bromo-1,2-dihydro-
  - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
    - (preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)
- RN 304854-04-4 HCAPLUS
- CN Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one, 6-bromo- (9CI) (CA INDEX NAME)

- L119 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN
- AN 2001:167971 HCAPLUS
- DN 134:207727
- ED Entered STN: 09 Mar 2001
- TI Preparation of quinolinones and related bicyclic compounds as androgen and progesterone receptor modulators.
- IN Zhi, Lin; Tegley, Christopher; Pio, Barbara; Arjan van Oeveren, Cornelis; Motamedi, Mehrnouch; Martinborough, Esther; West, Sarah; Higuchi, Robert; Hamann, Lawrence; Farmer, Luc
- PA Ligand Pharmaceuticals Incorporated, USA
- SO PCT Int. Appl., 356 pp.
  - CODEN: PIXXD2
- DT Patent
- LA English
- IC ICM C07D215-00
- CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
   Section cross-reference(s): 1, 63

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	PATENT NO.						KIN	D	DATE APPLICATION NO.						D	DATE				
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ΡI	WO	200	10	161	80		A2		2001	0308		WO 2	000-1	US23.	585		2	0000	825 <	
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AB Title compds., e.g. [I; R1, R2 = COR3, CSR3, SO2R3, NO, NR3R4, alkyl, alkenyl, haloalkyl, haloalkenyl, haloalkynyl, heteroalkyl, heteroalkenyl, heteroalkynyl, etc.; R1R2 = atoms to form (substituted) heterocyclyl; R3,

R4 = H, (substituted) alkyl, alkenyl, alkynyl, haloalkyl, heteroalkyl, heteroaryl, aryl; R5 = H, F, Cl, Br, iodo, OR3, SR3, NR3R4, alkyl, haloalkyl, heteroalkyl; R6 = F, Cl, Br, iodo, Me, CF3, CHF2, cyano, CF2Cl, CF2OR3, OR3, SOR3, CO2R3, NR3R4, (substituted) alkyl, alkenyl, alkynyl, haloalkyl, heteroalkyl, etc.; R7, R8 = H, F, Cl, Br, iodo, cyano, OR3, NR3R4, SR3, SOR3, NR3COR4, alkyl, haloalkyl, heteroalkyl, etc.; R9 = H, F, Cl, iodo, OR3, NR3R4, SR3, SOR3, SO2R3, alkyl, haloalkyl, heteroalkyl; R10 = NR1R2, (substituted) heterocyclyl; Y = O, S, NR3, NOR3, CR3R4], were prepared Thus, 6-amino-4-trifluoromethyl-2(1H)-quinolinone (preparation given) was stirred with propionaldehyde and NaBH3CN in MeOH to give 70-95% 6-propylamino-4-trifluoromethyl-2(1H)-quinolinone. The latter showed androgen receptor agonist activity with a potency of 27 nM. A drug composition is given.

- ST quinolinone prepn androgen progesterone receptor modulator
- IT Androgen receptors

### Progesterone receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process) (modulators; preparation of quinolinones and related bicyclic

compds. as androgen and progesterone receptor

modulators)

IT

IT

328947-93-9P 328951-07-1P 328955-28-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

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    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of quinolinones and related bicyclic compds. as androgen and
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    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of quinolinones and related bicyclic compds. as androgen and
        progesterone receptor modulators)
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    59-48-3, 2-Indolone 62-53-3, Aniline, reactions
                                                        64-19-7, Acetic acid,
                 67-64-1, Acetone, reactions
                                               70-34-8, 2,4-
    reactions
    Dinitrofluorobenzene
                            75-07-0, Acetaldehyde, reactions
                     75-89-8, 2,2,2-Trifluoroethanol
    2-Iodopropane
                                                       75-90-1,
                             75-98-9, Trimethylacetic acid
    Trifluoroacetaldehyde
                                                             76-03-9,
                                      76-04-0, Chlorodifluoroacetic acid
    Trichloroacetic acid, reactions
    76-05-1, Trifluoroacetic acid, reactions
                                                78-84-2, Isobutyraldehyde
                                      78-95-5, Chloroacetone
    78-93-3, 2-Butanone, reactions
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                        79-31-2, Isobutyric acid
    Bromoacetic acid
                                                   79-43-6, Dichloroacetic
                       79-44-7, Dimethylcarbamoyl chloride
    acid, reactions
                                                              91-21-4,
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                                                92-67-1, 4-Phenylaniline
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    97-52-9, 2-Amino-5-nitroanisole
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    Benzoyl chloride
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    4-Bromoaniline
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123-38-6, Propionaldehyde, reactions

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328956-55-4 328956-56-5 328956-60-1, 3-Fluoro-5-formylbenzeneboronic acid 328956-62-3 328956-63-4 328956-70-3 328956-71-4 328956-73-6
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

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(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

IT 328954-75-2P

IT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

RN 328954-75-2 HCAPLUS

CN 2H-3,1-Benzoxazine-2-thione, 6-(1-cyclohexen-1-yl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

L119 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:790489 HCAPLUS

DN 133:350229

ED Entered STN: 10 Nov 2000

TI Novel cyclocarbamate derivatives as progesterone receptor modulators

IN Zhang, Puwen; Terefenko, Eugene A.; Fletcher, Horace,
 III; Fensome, Andrew; Wrobel, Jay E.; Zhi, Lin; Jones, Todd K.;
 Marschke, Keith B.; Tegley, Christopher M.

PA American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SO PCT Int. Appl., 135 pp. CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D265-18

28-13 (Heterocyclic Compounds (More Than One Hetero Atom)) CC Section cross-reference(s): 1, 2 FAN.CNT 1 DATE DATE APPLICATION NO. PATENT NO. KIND ---------------\_\_\_\_\_\_ ----20000501 <--PΙ WO 2000066571 A1 20001109 WO 2000-US11822 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 6509334 В1 20030121 US 2000-552633 20000419 <---20001109 CA 2000-2371726 20000501 <--CA 2371726 AA EP 1173426 Αĺ 20020123 EP 2000-928689 20000501 <--AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO 20020219 BR 2000-10213 20000501 <--BR 2000010213 Α TR 2001-200103286 20000501 <--T2 20020722 TR 200103286 T2 20021217 JP 2000-615601 20000501 <--JP 2002543193 AU 766428 · B2 20031016 AU 2000-46886 20000501 <--NZ 2000-515355 20000501 <--20040227 NZ 515355 Α US 2001-948309 20010906 <--20020425 US 2002049204 A1 B2 . 20030520 US 6566358 , A 20020514 ZA 2001-7630 20010917 <--ZA 2001007630 Α 20020103 NO 2001-5378 20011102 <--NO 2001005378 BG 2001-106079 BG 106079 Α 20020531 20011102 <--US 2003-386799 20030312 <--US 2003216388 A1 20031120 B2 20040330 US 6713478 20040129 <--US 2004-767813 20040923 US 2004186101 A1 19990504 <--PRAI US 1999-183012P P 20000419 **A1** <--US 2000-552633 W 20000501 WO 2000-US11822 <--US 2001-948309 A3 20010906 <--A1 · 20030312 US 2003-386799 CLASS PATENT FAMILY CLASSIFICATION CODES CLASS PATENT NO. \_\_\_\_\_\_ ----WO 2000066571 ICM C07D265-18 C07D413-04; C07D417-04; C07D413-10; A61K031-536; ICS A61P015-00; A61P035-00 C07D265/18B; C07D413/04+265+213; C07D413/04+265+207; WO 2000066571 ECLA C07D413/04+307B+265; C07D413/04+333B+265; C07D413/10+265+257; C07D417/04+285B+265 514/230.500; 514/080.000; 514/183.000; 514/211.150; US 6509334 NCL 514/212.020; 514/217.050; 514/228.200; 540/466.000; 540/467.000; 540/481.000; 540/543.000; 540/544.000; 540/545.000; 540/599.000; 544/058.600; 544/069.000; 544/070.000; 544/092.000 C07D265/18B; C07D413/04+265+207; C07D413/04+265+213; **ECLA** C07D413/04+307B+265; C07D413/04+333B+265; C07D413/10+265+257; C07D417/04+285B+265 C07D265/18B; C07D413/04+265+207; C07D413/04+265+213; CA 2371726 **ECLA** C07D413/04+307B+265; C07D413/04+333B+265; C07D413/10+265+257; C07D417/04+285B+265 514/230.500; 514/212.020; 514/212.080; 514/228.200 US 2002049204 NCL C07D265/18B; C07D413/04+265+207; C07D413/04+265+213; ECLA

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                        C07D413/10+265+257; C07D417/04+285B+265
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AB This invention discloses novel aryl fused cyclocarbamate derivs. I (R1 or R2 = H, (un) substituted C1-6 alkyl, (un) substituted C2-6 alkenyl, (un) substituted C2-6 alkynyl, (un) substituted C3-8 cycloalkyl, (un) substituted aryl, (un) substituted heterocyclyl, amino derivative or R1 and R2 may be fused to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un) substituted C1-6 alkyl, (un) substituted C3-6 alkenyl, (un) substituted alkynyl, or COR6 {R6 = H, (un) substituted C1-3 alkyl, (un) substituted aryl, (un) substituted C1-3 alkoxy, or (un) substituted C1-3 aminoalkyl}; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, (un) substituted alkynyl, (un) substituted C1-6 alkoxy, amino, or (un) substituted C1-6 aminoalkyl; R5 = trisubstituted benzene ring or a five- or six-membered ring with 1, 2, or 3 heteroatoms selected from 0, S, SO, SO2 or NR7 and containing one or two independent substituents from the group including H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, or NR9COR8 {R7 = H or C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3
alkoxy or (un)substituted C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl ) or pharmaceutically acceptable salts thereof, as well as pharmaceutical compns. and methods using the compds. as antagonists of the progesterone receptor. Thus, cyclocarbamate II was prepared from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. Compds. of the invention demonstrated potency in the range of 0.01 nM to 5  $\mu M$  in the in vitro assays, and 0.001 to 300 mg/kg in the in vivo assays.

ST cyclocarbamate aryl prepn progesterone receptor modulator; benzooxazinone prepn progesterone receptor antagonist; oxazinone benzo prepn progesterone receptor antagonist

IT Progestogens

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU

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(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (antiprogestins; preparation of benzooxazinone derivs. as
        progesterone receptor modulators)
IT
    Antitumor agents
     Contraceptives
        (preparation of benzooxazinone derivs. as progesterone
        receptor modulators)
IT
     Progestogens
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of benzooxazinone derivs. as progesterone
        receptor modulators)
IT
     Progesterone receptors
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (preparation of benzooxazinone derivs. as progesterone
        receptor modulators)
IT
        (regulation of; preparation of benzooxazinone derivs. as
        progesterone receptor modulators)
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     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of benzooxazinone derivs. as progesterone
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     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of benzooxazinone derivs, as progesterone
        receptor modulators)
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108-36-1, 1,3-Dibromobenzene

100-58-3, Phenylmagnesium bromide

IT

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110-52-1, 1,4-Dibromobutane
                                   111-24-0, 1,5-Dibromopentane
     Triethylorthoformate 326-66-9, 4'-Bromo-2'-fluoroacetanilide
     1-Bromo-3,4-difluorobenzene
                                   460-00-4, 1-Bromo-4-fluorobenzene
     461-96-1, 1-Bromo-3,5-difluorobenzene 623-49-4, Ethylcyano formate
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- (1) Dong A Pharm Co Ltd; EP 0510235 A 1992 HCAPLUS
- (2) Du Pont Merck Pharma; WO 9814436 A 1998 HCAPLUS
- (3) Ligand Pharm Inc; WO 9619458 A 1996 HCAPLUS
- (4) Ligand Pharm Inc; US 5688810 A 1997 HCAPLUS
- (5) Merck & Co Inc; WO 9520389 A 1995 HCAPLUS

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RE

L119 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN AN2000:790488 HCAPLUS DN 133:350228 Entered STN: 10 Nov 2000 ED ΤI Preparation of cyclothiocarbamate derivatives as progesterone receptor modulators IN Zhang, Puwen; Fensome, Andrew; Terefenko, Eugene A.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher PA American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc. SO PCT Int. Appl., 101 pp. CODEN: PIXXD2 DTPatent LA English IC ICM C07D265-18 ICS C07D413-04; A61K031-536; A61P015-00; A61P035-00 28-13 (Heterocyclic Compounds (More Than One Hetero Atom)) Section cross-reference(s): 2 FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE . **---**---\_\_\_\_\_\_ ----------WO 2000066570 WO 2000-US11749 PΙ A1 20001109 20000501 <--AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 6436929 20020820 US 2000-552354 В1 20000419 <--CA 2371712 20001109 CA 2000-2371712 AΑ 20000501 <--EP 2000-930266 EP 1175411 A1 20020130 20000501 <--

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JP 2002543192

AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

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JP 2000-615600

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GΙ

$$R^{5}$$
 $R^{1}$ 
 $Q^{2}$ 
 $R^{4}$ 
 $R^{1}$ 
 $Q^{2}$ 

The title compds. [I or II; R1, R2 = H, alkyl, alkenyl, etc.; or R1 and R2 are fused to form (un)substituted 3-8 membered spiro cyclic alkyl or alkenyl ring or a spiro cyclic ring containing 1-3 heteroatoms selected from O, S and N; R3 = H, OH, NH2, etc.; R4 = H, halo, CN, etc.; R5 = (un)substituted Ph, 5-6 membered heterocyclic ring with 1-3 ring heteroatoms, 3-pyridyl, 5-pyrimidinyl; Q1 = S, NR7, CR8R9; R7 = CN, alkyl, cycloalkyl, etc.; R8, R9 = H, alkyl, cycloalkyl, etc.; Q2 = NR11OR12, NR11NR12R13, ONR11R13; R11-R13 = H, alkyl, aryl, etc.] which are agonists of the progesterone receptor, and are useful for contraception and the treatment of progesterone-related maladies, were prepared E.g., a multi-step synthesis of I [R1, R2 = Me; R3, R4 = H; R5 = 3-ClC6H4; Q1 = S] which showed EC50 of 0.65 nM against hPR in CV-1 cells, was given.

ST cyclothiocarbamate prepn progesterone receptor modulator; benzoxazinthione prepn progesterone receptor modulator

IT Contraceptives

(inducing contraception; preparation of cyclothiocarbamate derivs. as progesterone receptor modulators)

Progesterone receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)

(preparation of cyclothiocarbamate derivs. as progesterone

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receptor modulators)
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     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
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        (preparation of cyclothiocarbamate derivs. as progesterone
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    460-00-4, 1-Bromo-4-fluorobenzene 461-96-1, 1-Bromo-3,5-difluorobenzene
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        (preparation of cyclothiocarbamate derivs. as progesterone
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receptor modulators)
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclothiocarbamate derivs. as progesterone receptor modulators)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD RE

- (1) Dong A Pharm Co Ltd; EP 0510235 A 1992 HCAPLUS
- (2) Du Pont Merck Pharma; WO 9814436 A 1998 HCAPLUS
- (3) Ligand Pharm Inc; WO 9619458 A 1996 HCAPLUS
- (4) Ligand Pharm Inc; US 5688810 A 1997 HCAPLUS
- (5) Merck & Co Inc; WO 9520389 A 1995 HCAPLUS
- IT 304853-32-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclothiocarbamate derivs. as progesterone

receptor modulators)

RN 304853-32-5 HCAPLUS

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

L119 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2005 ACS on STN.

AN 2000:790347 HCAPLUS

DN 133:350205

ED Entered STN: 10 Nov 2000

TI Contraceptive compositions containing antiprogestinic and progestinic dihydro-2H-3,1-benzoxazin-2-ones

IN Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.

PA American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SO PCT Int. Appl., 146 pp. CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K045-06

ICS A61K031-57; A61K031-565; A61P015-18; A61K031-57; A61K031-535;

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A61K031-565; A61K031-565; A61K031-535; A61K031-565
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$$R^{1}$$
  $R^{2}$   $R^{2}$   $R^{3}$   $R^{4}$   $R^{3}$   $R^{3}$   $R^{4}$   $R^{4}$   $R^{5}$   $R^{4}$   $R^{5}$   $R^{6}$   $R^{6$ 

ST

AΒ The dihydrobenzoxazinones I [R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, acyl, acylamino; or R1R2 are fused to form spirocyclic or hetero-spirocyclic rings substituted by F, alkyl, alkoxy, alkylthio, F3C, HO, cyano, H2N, alkylamino; R3 = H, OH, NH2, C1-6 alkyl, C3-6 alkenyl, alkynyl, CORC; RC = H, C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, cyano, NO2, alkyl, alkynyl, alkoxy, alkoxy, amino, aminoalkyl; R5 = XYZC6H2, X = halo, cyano, alkyl, alkenyl, alkynyl, alkoxy, thioalkoxy, H2N, aminoalkyl, NO2, perfluoroalkyl, 5- or 6-membered heterocyclyl; Y, Z = H, halo, cyano, NO2, H2N, aminoalkyl, alkoxy, alkyl, thioalkoxy; or R5 = 5- or 6-membered heterocyclyl with O, S, SO, SO2 heteroatoms substituted by H, halo, cyano, NO2, H2N, alkyl, alkoxy, perfluoroacyl, perfluoroacylamino] and their pharmaceutically acceptable salts were prepared as antagonists of the progesterone receptor and were useful to induce contraception in mammals in cyclic combination therapies using an antiprogestin and progestin where the progestin is administered in the alternating presence and absence of an antiprogestin. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects of cyclic menstrual bleeding. Addnl. uses of the invention include stimulation of food intake. cyclocondensation of 2-(2-amino-5-bromophenyl)-2-propanol with carbonyldiimidazole gave the dimethylbenzoxazinone II which coupled with 3-chlorophenylboronic acid in DME/H2O containing (Ph3P)4Pd and Na2CO3 to give the (chlorophenyl) benzoxazinone III.

menstrual bleeding side effect treatment dihydrobenzoxazinone prepn; prostate carcinoma treatment dihydrobenzoxazinone prepn; colon carcinoma treatment dihydrobenzoxazinone prepn; breast carcinoma treatment dihydrobenzoxazinone prepn; ovary carcinoma treatment dihydrobenzoxazinone prepn; endometrium carcinoma treatment dihydrobenzoxazinone prepn; polycystic ovary treatment dihydrobenzoxazinone prepn; endometriosis treatment dihydrobenzoxazinone prepn; uterine leiomyomata treatment dihydrobenzoxazinone prepn; amenorrhea secondary treatment dihydrobenzoxazinone prepn; progesterone receptor antagonist dihydrobenzoxazinone prepn; benzoxazinone dihydro prepn contraceptive

Progesterone receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
(Biological study); PROC (Process)

(antagonists; preparation of substituted dihydrobenzoxazinones with

progesterone receptor antagonist activity for use in contraceptive compns.)

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IT Progestogens
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RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(antiprogestins; preparation of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

### IT Contraceptives

IT

(preparation of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

51-98-9, Norethindrone acetate 68-22-4, Norethindrone 427-51-0. 797-63-7, Levonorgestrel Cyproterone acetate 6533-00-2, Norgestrel 35189-28-7, Norgestimate 53016-31-2, 17-Deacetylnorgestimate 54048-10-1, 3-Ketodesogestrel 54024-22-5, Desogestrel 58691-88-6, Nomegestrol 60282-87-3, Gestodene 65928-58-7, Dienogest 67392-87-4, 105149-04-0, Osaterone Drospirenone 74513-62-5, Trimegestone RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(preparation of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

IT 304853-29-0P 304853-30-3P 304854-07-7P 304854-08-8P 304854-49-7P 305800-19-5P 305800-20-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

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304853-28-9P
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304854-21-5P
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305800-72-0P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

IT 100-58-3, Phenylmagnesium bromide 107-30-2, Chloromethyl methyl ether 108-36-1, 1,3-Dibromobenzene 110-52-1, 1,4-Dibromobutane 111-24-0, 1,5-Dibromopentane 122-51-0, Triethyl orthoformate 326-66-9 348-61-8, 1-Bromo-3,4-difluorobenzene 460-00-4, 1-Bromo-4-fluorobenzene 461-96-1, 1-Bromo-3,5-difluorobenzene 623-49-4, Ethyl cyanoformate

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625-92-3, 3,5-Dibromopyridine 814-49-3, Diethyl chlorophosphate
     1066-54-2, (Trimethylsilyl)acetylene 1072-85-1, 1-Bromo-2-fluorobenzene
     1072-97-5, 2-Amino-5-bromopyridine 1073-06-9, 1-Bromo-3-fluorobenzene
     1191-95-3, Cyclobutanone
                               1435-51-4, 1,3-Dibromo-5-fluorobenzene
     1546-79-8, 1-(Trifluoroacetyl)imidazole
                                               1589-82-8, Benzylmagnesium
     bromide
               1611-92-3, 3,5-Dibromotoluene
                                               1679-18-1, 4-Chlorophenylboronic
            1730-25-2, Allylmagnesium bromide
     acid
                                               2357-52-0, 4-Bromo-2-
     fluoroanisole
                     3177-80-8, 2-Amino-3-methoxybenzoic acid
     2-Chlorophenylboronic acid
                                  4301-14-8, Ethynylmagnesium bromide
     4333-56-6, Cyclopropyl bromide
                                      4692-98-2, 5-Bromoisatoic anhydride
     4701-17-1
                 4915-06-4, 5-Bromo-2-furancarbonitrile
                                                          5419-55-6,
     Triisopropyl borate
                          5794-88-7, 2-Amino-5-bromobenzoic acid
     3-Thiopheneboronic acid
                              6638-79-5, N,O-Dimethylhydroxylamine
     hydrochloride
                     6952-59-6, 3-Bromobenzonitrile
                                                      7087-65-2
                                                                  10365-98-7,
     (3-Methoxyphenyl)boronic acid
                                     13331-27-6, 3-Nitrophenylboronic acid
     14282-76-9, 2-Bromo-3-methylthiophene
                                            16466-97-0, 1-Propynylmagnesium
               18242-39-2, 1-Bromo-3,5-dinitrobenzene
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     18792-00-2
                  19472-74-3, 2-Bromophenylacetonitrile
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     29578-39-0
                  31938-07-5, 3-Bromophenylacetonitrile
                                                          33743-87-2
     33863-76-2
                  35590-37-5, 3-Bromo-5-cyanopyridine
                                                        51437-00-4
                                           53595-65-6
     53119-61-2, 2-Bromo-3-ethylthiophene
                                                         56182-43-5
                 63503-60-6, (3-Chlorophenyl)boronic acid
     60811-21-4
                                                             65854-91-3
     67492-50-6, 3,5-Dichlorophenylboronic acid
                                                  69249-60-1
                                                               73852-19-4
     79630-23-2
                  89599-01-9
                               105942-08-3
                                             112575-11-8
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                                         145543-82-4
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     5-Bromoisophthalonitrile
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     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of substituted dihydrobenzoxazinones with progesterone receptor
        antagonist activity for use in contraceptive compns.)
     2160-62-5P, 5-Bromo-2-thiophenecarbonitrile
                                                   2160-63-6P
                                                                21440-97-1P
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                                   305800-71-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of substituted dihydrobenzoxazinones with progesterone receptor
        antagonist activity for use in contraceptive compns.)
     304857-58-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of substituted dihydrobenzoxazinones with progesterone receptor
        antagonist activity for use in contraceptive compns.)
RE.CNT
              THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
```

- (1) Akzo Nobel Nv; WO 9749407 A 1997 HCAPLUS
- (2) Balance Pharmaceuticals Inc; WO 9615794 A 1996 HCAPLUS
- (3) Grubb, G; US 5521166 A 1996 HCAPLUS

IT

TT

RE

(4) Schering Ag; DE 4330234 A 1995 HCAPLUS

- (5) Schering Ag; DE 4344463 A 1995 HCAPLUS
- (6) Schneider, M; US 5733902 A 1998 HCAPLUS
- IT 304854-04-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

- RN 304854-04-4 HCAPLUS
- CN Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one, 6-bromo- (9CI) (CA INDEX NAME)

### => => d l113 all fhitstr tot

L113 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:475543 HCAPLUS

DN 133:105042

- ED Entered STN: 14 Jul 2000
- TI Preparation of 2-amino-4H-3,1-benzoxazin-4-one derivatives for the treatment of obesity
- IN Hodson, Harold Francis; Downham, Robert; Mitchell, Timothy John; Carr, Beverley Jane; Dunk, Christopher Robert; Palmer, Richard Michael John
- PA Alizyme Therapeutics Limited, UK
- SO PCT Int. Appl., 70 pp. CODEN: PIXXD2

DT Patent

- LA English
- IC ICM A61K031-536

ICS A61P003-04; C07D265-24; C07D498-04; C07D413-12; C07D498-04; C07D265-00; C07D221-00

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))

FAN.CNT 1 PATENT NO. DATE APPLICATION NO. KIND DATE ----------\_ \_ \_ \_ \_\_\_\_\_ -----PΙ 20000713 WO 2000-GB32 20000106 <--WO 2000040247 A1 20021024 WO 2000040247 C2 W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG CA 2000-2359819 20000106 <--CA 2359819 AA20000713 EP 2000-900082 EP 1143977 20011017 20000106 <--Α1 EP 1143977 20050420 B1

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     JP 2002534388
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                                                                      20000106 <--
                                             ZA 2000-3398
     ZA 2000003398
                           Α
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                                                                      20000706 <--
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                           C2
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                                             RU 2001-123171
                                                                      20010106 <--
     NO 2001003381
                           Α
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                                             NO 2001-3381
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     US 2003027821
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                                 20030206
                                             US 2001-901887
                                                                      20010706 <--
     US 6624161
                           B2
                                 20030923
     US 2003195206
                           Α1
                                 20031016
                                             US 2002-306377
                                                                      20021127 <--
PRAI GB 1999-413
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                                 19990108
                                           <--
     GB 1999-17294
                           Α
                                 19990722
                                            <--
     WO 2000-GB32
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     US 2001-901887
                           A3
                                 20010706
                                           <--
CLASS
PATENT NO.
                 CLASS PATENT FAMILY CLASSIFICATION CODES
 WO 2000040247
                 ICM
                         A61K031-536
                         A61P003-04; C07D265-24; C07D498-04; C07D413-12;
                 ICS
                         C07D498-04; C07D265-00; C07D221-00
WO 2000040247
                 ECLA
                         C07C271/28; C07D265/26B
US 2003027821
                         514/230.500; 544/093.000; 544/094.000
                 NCL
                 ECLA
                         C07C271/28; C07D265/26B.
US 2003195206
                 NCL
                         514/230.500
                 ECLA
                         C07C271/28; C07D265/26B
os
     MARPAT 133:105042
GI
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AB The title compds. I [A = 6-membered aromatic or heteroarom. ring; R1 = branched or unbranched alkyl (optionally interrupted by one or more oxygen atoms), alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl, arylalkyl, reduced arylalkyl, arylalkenyl, heteroaryl, heteroarylalkyl, heteroarylalkenyl, reduced aryl, reduced heteroarylalkyl, useful in the treatment of obesity, were prepared E.g., 2-phenylamino-4H-3,1-benzoxazin-4-one was prepared I were tested as inhibitors of pancreatic lipase.

ST aminobenzoxazinone prepn obesity treatment; benzoxazinone amino prepn obesity treatment

IT Antiobesity agents

(preparation of aminobenzoxazinones for the treatment of obesity) IT 945-04-0P 1026-16-0P 54722-44-0P 81905-02-4P 86672-55-1P 86672-56-2P 86672-60-8P 278609-56-6P 282529-85-5P 282529-86-6P 282529-90-2P 282529-87-7P 282529-88-8P 282529-89-9P 282529-91-3P 282529-92-4P 282529-93-5P 282529-94-6P 282529-96-8P 282529-97-9P 282529-98-0P 282530-00-1P 282530-01-2P 282530-03-4P 282530-05-6P 282530-07-8P 282530-08-9P 282530-09-0P 282530-11-4P 282530-13-6P 282530-14-7P 282530-16-9P 282530-17-0P 282530-18-1P 282530-20-5P 282530-22-7P 282530-24-9P 282530-26-1P 282530-28-3P 282530-30-7P

282530-32-9P 282530-33-0P 282530-35-2P 282530-36-3P 282530-37-4P 282530-39-6P 282530-40-9P 282530-42-1P 282530-43-2P 282530-49-8P 282530-47-6P 282530-51-2P 282530-53-4P 282530-55-6P 282530-57-8P 282530-59-0P 282530-61-4P 282530-62-5P 282530-64-7P 282530-66-9P 282530-68-1P 282530-69-2P 282530-70-5P 282530-73-8P 282530-74-9P · 282530-75-0P 282530-76-1P 282530-77-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of aminobenzoxazinones for the treatment of obesity) IT 9001-62-1 RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process) (preparation of aminobenzoxazinones for the treatment of obesity) IT 2305-36-4, 2-Amino-4-methylbenzoic acid 2909-38-8, 3-Chlorophenyl 2941-78-8, 2-Amino-5-methylbenzoic acid isocyanate 51554-93-9 59377-19-4, 4-Phenoxyphenyl isocyanate 132586-17-5 282530-78-3 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of aminobenzoxazinones for the treatment of obesity) IT 282526-99-2P 282527-00-8P 282527-03-1P 282527-01-9P 282530-83-0P 282530-84-1P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of aminobenzoxazinones for the treatment of obesity) RE.CNT THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) Bayer Ag; DE 2315303 A 1974 HCAPLUS (2) GUtschow, M; BIOORGANIC & MEDICINAL CHEMISTRY 1997, V5(10), P1935 HCAPLUS (3) Jarvest, R; BIOORGANIC & MEDICINAL CHEMISTRY LETTERS 1996, V6(20), P2463 HCAPLUS (4) Searle & Co; WO 9637485 A 1996 HCAPLUS (5) Syntex Inc; US 4657893 A HCAPLUS (6) Syntex Inc; EP 0147211 A 1985 HCAPLUS (7) Ulrich, H; US 3450700 A 1969 HCAPLUS (8) Warner Lambert Co; US 5652237 A HCAPLUS (9) Warner Lambert Co; WO 9607648 A 1996 HCAPLUS IT 282530-42-1P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminobenzoxazinones for the treatment of obesity) RN 282530-42-1 HCAPLUS

CN 4H-3,1-Benzoxazin-4-one, 6-cyclopropyl-2-(phenylamino)- (9CI) (CA INDEX NAME)

L113 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:213099 HCAPLUS

DN 118:213099

ED Entered STN: 29 May 1993

TI Imidazole-substituted benzoxazine and benzothiazine derivatives

```
IN
    Kim, Moohi Y.; Shin, Hyun T.; Lee, Choon W.; Kim, Joon W.; Kim, Soon H.;
    Choi, Youngmoon; Son, Moon H.
PA
    Dong-A Pharm. Co., Ltd., S. Korea
    U.S., 12 pp.
so
    CODEN: USXXAM
DT
    Patent
    English
LA
TC
    ICM C07D413-02
    ICS C07D413-10; C07D417-02; C07D417-10
INCL 544050000
    28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
    Section cross-reference(s): 1
FAN.CNT 1
    PATENT NO.
                       KIND
                              DATE
                                         APPLICATION NO.
                                                               DATE
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                                         -----
                                                               -----
PΙ
    US 5171851
                        Α
                              19921215
                                         US 1991-674183
                                                               19910325 <--
    KR 164842
                        B1
                              19990115
                                         KR 1990-3989
                                                               19900324 <--
    JP 04217977
                        A2
                                         JP 1991-82966
                              19920807
                                                               19910325 <--
PRAI KR 1990-3989
                        Α
                              19900324
CLASS
PATENT NO.
               CLASS PATENT FAMILY CLASSIFICATION CODES
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US 5171851
                ICM
                      C07D413-02
                ICS
                      C07D413-10; C07D417-02; C07D417-10
                INCL
                      544050000
US 5171851
               NCL
                      544/050.000; 544/092.000
                                                                       <--
OS
    CASREACT 118:213099; MARPAT 118:213099
GI
```

Ι

Title compds. I (X, X1 = 0, S; R-R2 = H, alkyl; R1R2 = CH:CHCH:CH) were prepared as cardiac stimulants. Thus, reduction of 2-amino-3-methyl-5-(4-methyl-1H-imidazol-1-yl)benzaldehyde gave 59% 2-amino-3-methyl-5-(4-methyl-1Himidazol-1-yl)benzyl alc. which was converted to the N-ethoxycarbonyl derivative Cyclocondensation of the latter gave 87% I (X, X1 = 0, R = Me, R1 = H, R2 = 4-Me, II). At 1.2  $\mu$ g II caused 30% increase in the contractile force of an isolated dog heart and a 5% increase in sinus stcardiotonic imidazolylbenzoxazine imidazolylbenzothiazine; benzoxazinone imidazolyl cardiotonic prepn; benzothiazinone imidazolyl cardiotonic prepn ΙT Cardiotonics (inotropics, (imidazolyl)benzoxazinones and -thiones, (imidazolyl)benzothiazinones and -thiones) IT 81840-03-1P 145622-93-1P 145622-94-2P 145622-95-3P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for (imidazolyl)benzoxazinone (inotropic)) IT 145622-96-4P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for (imidazoly1)benzoxazinone or

```
(imidazolyl)benzothiazinone (inotropic))
IT
     102791-88-8P
                    102791-94-6P
                                   147030-57-7P
                                                   147030-58-8P
                                                                  147030-59-9P
     147030-60-2P
                    147030-61-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, as intermediate for (imidazolyl)benzoxazinone or
        (imidazolyl)benzothiazinone derivative (inotropic))
ΙT
     145622-69-1P
                    145622-70-4P
                                   145622-71-5P
                                                   145622-72-6P
                                                                  145622-73-7P
     145622-74-8P
                    145622-75-9P
                                   145622-76-0P
                                                   145622-77-1P
                                                                  145622-78-2P
     145622-80-6P
                    145622-81-7P
                                   145622-82-8P
                                                   145622-83-9P
                                                                  145622-84-0P
     145622-85-1P
                    145622-86-2P
                                   145622-87-3P
                                                   145622-88-4P
                                                                  145622-89-5P
     145622-90-8P
                    145622-91-9P 145622-92-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, as pos. inotropic)
IT
     147017-49-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reactant for (imidazolyl)benzothiazinone (inotropic))
    140-89-6, Ethyl potassium xanthate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reactant for (imidazolyl)benzothiazinone derivative (inotropic))
IT
     693-98-1, 2-Methyl-1H-imidazole 6628-86-0, 5-Chloro-2-nitrobenzaldehyde
     147017-50-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reactant for (imidazolyl)benzoxazinone (inotropic))
     446-33-3, 5-Fluoro-2-nitrotoluene 822-36-6, 4-Methyl-1H-imidazole
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reactant for (imidazolyl)benzoxazinone or (imidazolyl)benzothiazinone
        derivative (inotropic))
TT
     147789-30-8
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with potassium Et xanthate, in preparation of inotropic
        cardiac stimulants)
    145622-92-0P
IT
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, as pos. inotropic)
RN
     145622-92-0 HCAPLUS
     2H-3,1-Benzoxazine-2-thione, 1,4-dihydro-8-methyl-6-(4-methyl-1H-imidazol-
CN
     1-yl) - (9CI) (CA INDEX NAME)
```

$$\begin{array}{c|c} Me & H \\ N & O \end{array}$$

```
L113 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
     1993:101972 HCAPLUS
AN
DN
     118:101972
ED
     Entered STN: 19 Mar 1993
TΤ
     Preparation of benzoxazinones, benzothiazinones, and related compounds as
     cardiotonics
IN
     Moohi, Yoo Kim; Hyun, Tae Shin; Choon, Woo Lee; Joon, Wan Kim; Soon, Hoe
     Kim; Youngmoon, Choi; Moon, Ho Son
PΑ
     Dong A Pharm. Co., Ltd., S. Korea
     Eur. Pat. Appl., 31 pp.
SO
     CODEN: EPXXDW
```

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DT
    Patent
LA
    English
IC
    ICM C07D413-04
    ICS C07D417-04; C07D471-04; A61K031-535; A61K031-54
    C07D233-58; C07D233-61
ICA
    C07D471-04, C07D235-00, C07D221-00
ICI
    28-14 (Heterocyclic Compounds (More Than One Hetero Atom))
CC
    Section cross-reference(s): 1
FAN.CNT 1
    PATENT NO.
                       KIND
                              DATE
                                         APPLICATION NO.
                                                               DATE
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                                         -----
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                                                                -----
    EP 510235
                        A1
                              19921028
                                         EP 1991-106822
                                                               19910426 <--
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
PRAI EP 1991-106822
                              19910426
                                       <--
CLASS
PATENT NO.
                CLASS PATENT FAMILY CLASSIFICATION CODES
                _ _ _ _ _
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EP 510235
                ICM
                      C07D413-04
                ICS
                      C07D417-04; C07D471-04; A61K031-535; A61K031-54
                ICA
                      C07D233-58; C07D233-61
                ICI
                      C07D471-04, C07D235-00, C07D221-00
os
    MARPAT 118:101972
GΙ
```

AB

methylimidazol-1-yl)benzyl carbonate (preparation starting from 5-chloro-2-nitrobenzaldehyde given) was stirred with NaOMe in MeOH at 0° to room temperature to give 75% title compound II. I increased contractility in blood-perfused dog papillary muscle preparation by 5.24-79.2% at 1-30 µq. imidazolylbenzoxazinone prepn cardiotonic; benzothiazinone imidazolyl ST cardiotonic; benzoxazinone imidazolyl cardiotonic IT Cardiotonics (imidazolylbenzoxazinones and -benzothiazinones and related compds.) 145622-70-4P 145622-72-6P 145622-71-5P IT 145622-69-1P 145622-73-7P 145622-75-9P 145622-77-1P 145622-76-0P 145622-74-8P 145622-78-2P 145622-81-7P 145622-79-3P 145622-80-6P 145622-82-8P 145622-83-9P 145622-87-3P 145622-84-0P 145622-85-1P 145622-86-2P 145622-88-4P 145622-90-8P 145622-91-9P 145622-92-0P 145622-89-5P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as cardiotonic) IT 81840-03-1P 102791-89-9P 102791-95-7P 145622-93-1P 145622-94-2P 145622-95-3P 145622-96-4P 145622-97-5P 145622-98-6P 145622-99-7P 145623-00-3P 145623-01-4P 145623-02-5P RL: SPN (Synthetic preparation); PREP (Preparation)

Title compds. (I; X, Y = O, S; R1-R3 = H, alkyl; R1R2 = atoms to form a

fused aromatic heterocycle) were prepared Thus, Et 2-ethoxycarbonylamino-5-(2-

(preparation of, as intermediate for imidazolylbenzoxazinone cardiotonic)

IT 140-89-6, Potassium ethyl xanthate 145623-03-6 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of imidazolylbenzothiazinone cardiotonic)

IT 6160-65-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of imidazolylbenzoxazinethione cardiotonic)

IT 541-41-3, Ethyl chloroformate 693-98-1, 2-Methylimidazole 822-36-6, 4-Methylimidazole 5367-28-2, 5-Chloro-2-nitrotoluene 6628-86-0, 5-Chloro-2-nitrobenzaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of imidazolylbenzoxazinone cardiotonic)

IT 145622-92-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as cardiotonic)

RN 145622-92-0 HCAPLUS

CN 2H-3,1-Benzoxazine-2-thione, 1,4-dihydro-8-methyl-6-(4-methyl-1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)

L113 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1989:95163 HCAPLUS

DN 110:95163

ED Entered STN: 17 Mar 1989

TI Studies on positive inotropic agents. VI. Synthesis of 1-aromatic ring substituted 4-(3,4-dimethoxybenzoyl)piperazine derivatives

AU Ogawa, Hidenori; Tamada, Shigeharu; Fujioka, Takafumi; Teramoto, Shuji; Kondo, Kazumi; Yamashita, Shuji; Yabuuchi, Youichi; Tominaga, Michiaki; Nakagawa, Kazuyuki

CS Tokushima Res. Inst., Otsuka Pharm. Co., Ltd., Tokushima, 771-01, Japan

SO Chemical & Pharmaceutical Bulletin (1988), 36(7), 2401-9 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

OS CASREACT 110:95163

GΙ

Ι

$$\begin{array}{c|c}
 & Z^2 \\
 & Z^1 \\
 & N \\
 & R^1
\end{array}$$
MeO
MeO
MeO

Piperazines I (R1 = H, Me; Z1 = S, O, NH, NMe; Z2 = H2, O; Z3 = S, O) were AB prepared, and they showed inotropic activity. A Me 5-(1pipeazinyl)anthranilate derivative was treated with MeNCO to give I (R1 = H, Z1 = NMe, Z2 = Z3 = O).piperazine heteroaryl prepn inotropic; inotropic ST heteroarylbenzoylpiperazine prepn IT Cardiotonics (inotropics, heteroaryl(dimethoxybenzoyl)piperazines) 407-25-0, Trifluoroacetic anhydride IT RL: RCT (Reactant); RACT (Reactant or reagent) (acylation by, of anthranilic acid derivative) IT 3535-37-3, 3,4-Dimethoxybenzoyl chloride RL: RCT (Reactant); RACT (Reactant or reagent) (acylation by, of piperazines) 74-88-4, reactions IT RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation by, of quinazolinedione derivative and anthranilic acid derivative) 13796-06-0, 5-Chloro-2-nitrobenzaldehyde dimethyl acetal RL: RCT (Reactant); RACT (Reactant or reagent) (arylation by, of piperazine) IT 51282-49-6, Methyl 5-chloro-2-nitrobenzoate RL: RCT (Reactant); RACT (Reactant or reagent) (arylation by, of piperazine derivative) IT 2759-28-6, 1-Benzylpiperazine RL: RCT (Reactant); RACT (Reactant or reagent) (arylation of, by chlorobenzoic acid derivative) IT 110-85-0, Piperazine, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (arylation of, by chloronitrobenzaldehyde derivative) IT 43204-63-3, Bis(2-bromoethyl)amine hydrobromide RL: RCT (Reactant); RACT (Reactant or reagent) (cycloalkylation by, of aminoindole and aminobenzothiazole derivs.) IT 20876-36-2 56354-98-4 RL: RCT (Reactant); RACT (Reactant or reagent) (cycloalkylation of, by bis(bromoethyl)amine) IT 140-89-6, Potassium ethyl xanthate RL: RCT (Reactant); RACT (Reactant or reagent) (cyclocondensation reaction of, with aminobenzyl alc. derivative) IT 76-02-8, Trichloroacetyl chloride RL: RCT (Reactant); RACT (Reactant or reagent) (cyclocondensation reaction of, with aminobenzyl alc. derivative, in preparation benzoxazinone derivative) IT 75-15-0, Carbon disulfide, reactions 75-44-5, Phosgene 7791-25-5, Sulfuryl chloride RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclocondensation reaction of, with aminobenzylamine derivative)

```
IT
     334-88-3, Diazomethane
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (esterification by, of anthranilic acid derivative)
     590-28-3, Potassium isocyanate 624-83-9, Methyl isocyanate
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (of cyclocondensation reaction of, with anthranilate ester derivative)
IT
     86813-46-9P
                   99111-45-2P
                                 102358-66-7P
                                                119198-22-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and acylation of, by benzoyl chloride derivative)
IT
     119198-29-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and conversion of, to anthranilate ester derivative)
IT
     81840-07-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and conversion of, to benzyl alc., benzoic acid and benzylamine
        analogs)
IT
     119198-33-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation reaction of, with potassium isocyanate)
IT
     119198-30-0P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation reactions of, with alkali and alkyl
        isocyanates)
IT
     119198-38-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation reactions of, with sulfuryl chloride,
        phosgene and carbon disulfide)
IT
     119198-24-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation reactions of, with xanthate ester and
        trichloroacetyl chloride)
IT
     119198-34-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and hydrogenolysis of)
IT
     99111-46-3P
                  102358-67-8P
                                 119198-23-1P
                                                 119198-25-3P
                                                  119198-31-1P
     119198-26-4P
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     119198-32-2P
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                                                                  119198-40-2P
     119198-41-3P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (preparation and inotropic activity of)
IT
     119198-45-7P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and methylation-deacylation of)
                    119198-42-4P
IT
     119198-37-7P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reduction of)
IT
     119198-43-5P
                   119198-44-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and trifluoroacetylation of)
```

IT 119198-26-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and inotropic activity of)

RN 119198-26-4 HCAPLUS

CN Piperazine, 1-(1,4-dihydro-2-thioxo-2H-3,1-benzoxazin-6-yl)-4-(3,4-dimethoxybenzoyl)- (9CI) (CA INDEX NAME)

#### => => d his l120-

## => fil uspatful

FILE 'USPATFULL' ENTERED AT 07:57:34 ON 05 JUL 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 5 Jul 2005 (20050705/PD)
FILE LAST UPDATED: 5 Jul 2005 (20050705/ED)
HIGHEST GRANTED PATENT NUMBER: US6915531
HIGHEST APPLICATION PUBLICATION NUMBER: US2005144692
CA INDEXING IS CURRENT THROUGH 5 Jul 2005 (20050705/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 5 Jul 2005 (20050705/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2005

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USPAT2 is now available. USPATFULL contains full text of the
>>>
                                                                       <<<
    original, i.e., the earliest published granted patents or
>>>
                                                                       <<<
    applications. USPAT2 contains full text of the latest US
                                                                       <<<
    publications, starting in 2001, for the inventions covered in
                                                                       <<<
    USPATFULL. A USPATFULL record contains not only the original
                                                                       <<<
>>> published document but also a list of any subsequent
                                                                       <<<
>>> publications. The publication number, patent kind code, and
                                                                       <<<
>>> publication date for all the US publications for an invention
                                                                       <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL
                                                                       <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
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>>> USPATFULL and USPAT2 can be accessed and searched together

>>> through the new cluster USPATALL. Type FILE USPATALL to

>>> /PK, etc.

<<<

<<<

<<<

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enter this cluster.
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>>>
                                                                        <<<
    Use USPATALL when searching terms such as patent assignees,
>>>
                                                                        <<<
>>> classifications, or claims, that may potentially change from
                                                                        <<<
>>> the earliest to the latest publication.
                                                                        <<<
This file contains CAS Registry Numbers for easy and accurate
substance identification.
=> d l125 bib abs hitrn fhitstr tot
L125 ANSWER 1 OF 10 USPATFULL on STN
AN
       2005:62604 USPATFULL
       Partially absorbable fiber-reinforced composites for controlled drug
ΤI
IN
       Shalaby, Shalaby W, Anderson, SC, UNITED STATES
PΙ
       US 2005053639
                         A1
                               20050310
ΑI
       US 2004-935808
                          A1
                               20040908 (10)
RLI
       Continuation-in-part of Ser. No. US 2004-860677, filed on 3 Jun 2004,
       PENDING
PRAI
       US 2003-482898P
                           20030626 (60)
      Utility
DT
FS
      APPLICATION
LREP
       LEIGH P. GREGORY, ATTORNEY AT LAW, PO BOX 168, CLEMSON, SC, 29633-0168
CLMN
      Number of Claims: 30
ECL.
       Exemplary Claim: 1
      No Drawings
DRWN
LN.CNT 774
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       This invention describes a partially absorbable, fiber-reinforced
       composite in the form of a ring, or a suture-like thread, with modified
       terminals for use as a controlled delivery system of at least one
       bioactive agent, wherein said composite comprising an absorbable fiber
       construct capable of providing time-dependent mechanical properties of a
       biostable elastomeric matrix containing an absorbable microparticulate
       ion-exchanger to modulate the release of the bioactive agent(s) for a
       desired period(s) of time at a specific biological site; this can be a
       vaginal canal, peritoneal cavity, scrotum, prostate gland, an ear loop
       or subcutaneous tissue. Such drug delivery systems can be used for the
       local administration of at least one bioactive agent, including those
       used as contraceptive, antimicrobial, anti-inflammatory and/or antiviral
       agents as well as for cancer treatment.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
     304853-42-7, Tanaproget
        (partially absorbable fiber-reinforced composites for controlled drug
        delivery)
   304853-42-7, Tanaproget
IT
        (partially absorbable fiber-reinforced composites for controlled drug
        delivery)
     304853-42-7 USPATFULL
RN
CN
     1H-Pyrrole-2-carbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-
       benzoxazin-6-yl)-1-methyl- (9CI) (CA INDEX NAME)
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L125 ANSWER 2 OF 10 USPATFULL on STN
AN
       2004:19494 USPATFULL
ΤI
       Cyclothiocarbamate derivatives as progesterone receptor modulators and
       methods of treating skin disorders
IN
       Fensome, Andrew, Wayne, PA, UNITED STATES
       Harrison, Diane Deborah, Villanova, PA, UNITED STATES
       Winneker, Richard Craig, Penllyn, PA, UNITED STATES
       Zhang, Puwen, Audubon, PA, UNITED STATES
       Kern, Jeffrey Curtis, Gilbertsville, PA, UNITED STATES
       Terefenko, Eugene Anthony, Quakertown, PA, UNITED STATES
PA
       Wyeth, Madison, NJ (U.S. corporation)
PΙ
       US 2004014798
                          A1
                               20040122
AΙ
       US 2003-601968
                               20030623 (10)
                          A1
PRAI
       US 2002-391885P
                           20020625 (60)
                                                                     < - -
DT
       Utility
       APPLICATION
FS
LREP
       HOWSON AND HOWSON, CATHY A. KODROFF, ONE SPRING HOUSE CORPORATE CENTER,
       BOX 457, SPRING HOUSE, PA, 19477
CLMN
       Number of Claims: 27
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 2498
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       The present invention provides methods of treating skin disorders
AB
       includes delivering to a mammal a composition containing a compound of
       formula I, or tautomers thereof, in a regimen, wherein formula I is:
       ##STR1##
       and wherein R.sup.1-R.sup.5 and Q.sup.1 are defined as described herein.
       Specifically, methods for treating acne, hirsutism, and conditioning the
       skin are described. Also provided are novel PR modulators of formula II.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
     638989-33-0P 638989-38-5P 638989-41-0P
      638989-44-3P 638989-46-5P 638989-48-7P
        (cyclothiocarbamate derivs. as progesterone receptor modulators and use
        thereof for treatment of skin disorders)
     304853-32-5 304853-35-8 304853-37-0
      304853-38-1 304853-39-2 304853-40-5
      304853-41-6 304853-42-7 304853-43-8
      304853-44-9 304853-45-0 304853-46-1
      304853-47-2 304853-48-3 304853-49-4
      304853-50-7 304853-51-8 304853-52-9
      304853-53-0 304853-54-1 304853-55-2
      304853-56-3 304853-57-4 304853-58-5
      304853-59-6 304853-60-9 304853-61-0
      304853-62-1 304853-63-2 304853-64-3
      304853-66-5 304853-67-6 304853-68-7
      304853-69-8 304853-70-1 304853-71-2
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304853-72-3 304853-73-4 304853-74-5 304853-75-6 304853-76-7 304853-77-8 304853-78-9 304853-80-3 304853-81-4 304853-82-5 304853-83-6 304853-84-7 304853-85-8 304853-86-9 304853-87-0 304853-88-1 304853-95-0

(cyclothiocarbamate derivs. as progesterone receptor modulators and use thereof for treatment of skin disorders)

#### IT 638989-33-0P

(cyclothiocarbamate derivs. as progesterone receptor modulators and use thereof for treatment of skin disorders)

RN 638989-33-0 USPATFULL

CN 1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

L125 ANSWER 3 OF 10 USPATFULL on STN

AN 2004:7820 USPATFULL

TI Methods of treating hormone-related conditions using cyclothiocarbamate derivatives

IN Fensome, Andrew, Wayne, PA, UNITED STATES
Grubb, Gary S., Newtown Square, PA, UNITED STATES
Harrison, Diane Deborah, Villanova, PA, UNITED STATES
Winneker, Richard Craig, Penllyn, PA, UNITED STATES
Zhang, Puwen, Audubon, PA, UNITED STATES
Kern, Jeffrey Curtis, Gilbertsville, PA, UNITED STATES

Kern, Jeffrey Curtis, Gilbertsville, PA, UNITED STATES Terefenko, Eugene Anthony, Quakertown, PA, UNITED STATES

PA Wyeth, Madison, NJ (U.S. corporation)

PI US 2004006060 A1 20040108

AI US 2003-601481 A1 20030623 (10)

PRAI US 2002-391871P 20020625 (60)

DT Utility

FS APPLICATION

LREP HOWSON AND HOWSON, CATHY A. KODROFF, ONE SPRING HOUSE CORPORATE CENTER, BOX 457, SPRING HOUSE, PA, 19477

CLMN Number of Claims: 28

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 2452

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides methods of inducing contraception which includes delivering to a female a composition containing a compound of formula I or formula II, or tautomers thereof, in a regimen which involves delivering one or more of a selective estrogen receptor modulator, wherein formula I is: ##STR1##

and wherein R.sup.1-R.sup.5 and Q.sup.1 are defined as described herein. Methods of providing hormone replacement therapy and for treating carcinomas, dysfunctional bleeding, uterine leiomyomata, endometriosis, and polycystic ovary syndrome is provided which includes delivering a

compound of formula I and a selective estrogen receptor modulator are also described.

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CAS INDEXING IS AVAILABLE FOR THIS PATENT.
     304853-32-5P, 6-(3-Chlorophenyl)-4,4-dimethyl-1,4-
     dihydrobenzo[d][1,3]oxazin-2-thione 304853-33-6P,
      4-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-
     yl)thiophene-2-carbonitrile 304853-35-8P, 3-(4,4-Dimethyl-2-
     thioxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)-5-fluorobenzonitrile
     304853-37-0P, 3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-
     benzo[d][1,3]oxazin-6-yl)benzonitrile 304853-38-1P,
      6-(3-Fluorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
      304853-39-2P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
     benzoxazin-6-yl)-4-methylthiophene-2-carbonitrile 304853-40-5P,
      5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-pyrrole-2-
      carbonitrile 304853-41-6P, [6-(4,4-Dimethyl-2-thioxo-1,4-
      dihydro-2H-3,1-benzoxazin-6-yl)pyridin-2-yl]acetonitrile
      304853-42-7P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
     benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile 304853-43-8P
      , 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-pyrrole-
      2-carbothioamide 304853-44-9P, 5-(4,4-Dimethyl-2-thioxo-1,4-
     dihydro-2H-benzo[d][1,3]oxazin-6-yl)thiophene-3-carbonitrile
      304853-45-0P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
     benzoxazin-6-yl)-1-ethyl-1H-pyrrole-2-carbonitrile 304853-46-1P
       4-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazin-4,1-cyclohexan]-6-yl]-2-
      thiophenecarbonitrile 304853-47-2P, 5-(4,4-Dimethyl-2-thioxo-
      1,4-dihydro-2H-3,1-benzoxazin-6-yl)-2-fluorobenzonitrile
      304853-48-3P, 6-(5-Bromopyridin-3-yl)-4,4-dimethyl-1,4-dihydro-2H-
      3,1-benzoxazine-2-thione 304853-49-4P, 6-(3-Chloro-5-
      fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
      304853-50-7P, 6-(3-Bromo-5-methylphenyl)-4,4-dimethyl-1,4-dihydro-
      2H-3,1-benzoxazine-2-thione 304853-51-8P, 6-(3-Bromo-5-
      trifluoromethoxyphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
      thione 304853-52-9P, 3-[1,2-Dihydro-2-thioxospiro[4H-3,1-
      benzoxazine-4,1-cyclohexan]-6-yl]-5-fluorobenzonitrile
      304853-53-0P, 3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
      benzoxazin-6-yl)-5-methylbenzonitrile 304853-54-1P,
      6-(3,5-Dichlorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
      thione 304853-56-3P, 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-
      3,1-benzoxazin-6-yl)-2-furonitrile 304853-57-4P,
      4,4-Diethyl-6-(3-nitrophenyl)-1,4-dihydro-2H-3,1-benzoxazine-2-thione
      304853-58-5P, 6-(3-Chlorophenyl)-4-methyl-4-phenyl-1,4-dihydro-2H-
      3,1-benzoxazine-2-thione 304853-59-6P, 4-Allyl-6-(3-
      chlorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
      304853-60-9P, 3-Chloro-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-
      3,1-benzoxazin-6-yl)benzonitrile 304853-61-0P,
      6-(3,5-Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
      thione 304853-62-1P, 6-(3-Fluoro-5-methoxyphenyl)-4,4-dimethyl-
      1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-63-2P,
      3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-5-
      methoxybenzonitrile 304853-64-3P, 6-(3-Fluorophenyl)-4,4-
      dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-65-4P,
      6-[3-Fluoro-5-(trifluoromethyl)phenyl]-4,4-dimethyl-1,4-dihydro-2H-3,1-
      benzoxazine-2-thione 304853-66-5P, 6-(2-Fluorophenyl)-4,4-
      dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-67-6P,
      6-(3,4-Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-
      thione 304853-68-7P, 6-(4-Fluorophenyl)-4,4-dimethyl-1,4-
      dihydro-2H-3,1-benzoxazine-2-thione 304853-69-8P,
      3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-4-
      fluorobenzonitrile 304853-70-1P, 6-(2,3-Difluorophenyl)-4,4-
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dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-71-2P,
  3-(8-Bromo-4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-5-
  fluorobenzonitrile 304853-72-3P, 4,4-Dimethyl-6-(3-nitrophenyl)-
  1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-73-4P,
  6-(3-Chlorophenyl)-4,4-diethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione
  304853-74-5P, 6-(3-Methoxyphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-
  benzoxazine-2-thione 304853-75-6P, 6-(2-Chlorophenyl)-4,4-
  dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-76-7P.
  4-Benzyl-6-(3-chlorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-
  thione 304853-77-8P, 6-(3-Bromo-5-fluorophenyl)-4,4-dimethyl-
  1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-78-9P,
  5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)thiophene-2-
  carbonitrile 304853-79-0P, 3-Fluoro-5-(8-fluoro-4,4-dimethyl-2-
  thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)benzonitrile
  304853-80-3P, 3-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-
  4,1'-cyclohexan]-6-yl]benzonitrile 304853-81-4P,
  5-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-4-
  methyl-2-thiophenecarbonitrile 304853-82-5P,
  5-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-2-
  thiophenecarbonitrile 304853-83-6P, 6-(3-Chloro-4-fluorophenyl)-
  4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione 304853-84-7p
  , 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-4-
  propylthiophene-2-carbonitrile 304853-85-8P,
  4-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-2-
  furonitrile 304853-86-9P, 4-Butyl-5-(4,4-dimethyl-2-thioxo-1,4-
  dihydro-2H-3, 1-benzoxazin-6-yl) thiophene-2-carbonitrile
  304853-87-0P, 6-(3-Bromophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-
  benzoxazine-2-thione 304853-88-1P, 2-(4,4-Dimethyl-2-thioxo-1,4-
  dihydro-2H-3,1-benzoxazin-6-yl)thiophene-3-carbonitrile
  304853-95-0P, 2-Cyano-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-
  benzoxazin-6-yl)-1H-pyrrole-1-carboxylic acid tert-Butyl ester
  638989-33-0P, 1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-
  benzoxazine-4,1'-cyclobutan]-6-yl]-1H-pyrrole-2-carbonitrile
  638989-38-5P, 5-(4,4-Diethyl-2-thioxo-1,4-dihydro-2H-3,1-
  benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile 638989-41-0P
    5-(4-\text{Ethyl}-4-\text{methyl}-2-\text{thioxo}-1,4-\text{dihydro}-2H-3,1-\text{benzoxazin}-6-\text{yl})-1-
  methyl-1H-pyrrole-2-carbonitrile 638989-44-3P,
  1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclohexan]-6-
  yl]-1H-pyrrole-2-carbonitrile 638989-46-5P,
  1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclopentan]-6-
  yl]-1H-pyrrole-2-carbonitrile 638989-48-7P,
  1-Methyl-5-[2-thioxo-4,4-bis(trifluoromethyl)-1,4-dihydro-2H-3,1-
  benzoxazin-6-yl]-1H-pyrrole-2-carbonitrile 639085-00-0P,
  5-(4,4-Dimethyl-1,2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-
  yl)isophthalonitrile
    (drug candidate; use of cyclothiocarbamate derivs. as selective
    androgen antagonists in contraception, hormone replacement therapy and
    in treatment of other hormone-related conditions)
304853-32-5P, 6-(3-Chlorophenyl)-4,4-dimethyl-1,4-
  dihydrobenzo[d][1,3]oxazin-2-thione
    (drug candidate; use of cyclothiocarbamate derivs. as selective
    androgen antagonists in contraception, hormone replacement therapy and
    in treatment of other hormone-related conditions)
 304853-32-5 USPATFULL
 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-
         (CA INDEX NAME)
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RN

CN

No Drawings

L125 ANSWER 4 OF 10 USPATFULL on STN AN 2003:277179 USPATFULL TТ 2-Oxy-benzoxazinone derivatives for the treatment of obesity TN Hodson, Harold Francis, Beckenham, UNITED KINGDOM Downham, Robert, Cambridge, UNITED KINGDOM Mitchell, Timothy john, Cambridge, UNITED KINGDOM Carr, Beverley Jane, Royston, UNITED KINGDOM Dunk, Christopher Robert, Ely, UNITED KINGDOM Palmer, Richard Michael John, Hayes, UNITED KINGDOM PΙ US 2003195206 **A1** 20031016 ΑI US 2002-306377 Α1 20021127 (10) RLI Division of Ser. No. US 2001-901887, filed on 6 Jul 2001, PENDING Continuation of Ser. No. WO 2000-GB32, filed on 6 Jan 2000, UNKNOWN PRAI GB 1999-413 19990108 GB 1999-17294 19990722 <--DT Utility FS APPLICATION LREP Choate, Hall & Stewart, Exchange Place, 53 State Street, Boston, MA, CLMN Number of Claims: 53 ECL Exemplary Claim: 1

or a salt, ester, amide or prodrug therof in the inhibition of an enzyme whose preferred mode of action is to catalyse the hydrolysis of an ester functionality, e.g. in the control and inhibition of unwanted enzymes in products and processes. The compounds are also useful in medicine e.g. in the treatment of obesity and related conditions. The invention also relates to novel compounds within formula (I), to processes for preparing them and pharmaceutical compositions containing them.

In formula (I) A is a 6-membered aromatic or heteroaromatic ring; and R.sup.1 is a branched or unbranched alkyl (optionally interrupted by one or more oxygen atoms), alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl, arylalkyl, reduced arylalkyl, arylalkenyl, heteroaryl, heteroarylalkyl, heteroarylalkenyl, reduced aryl, reduced heteroarylalkyl or a substituted derivative of any of the foregoing groups.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

The use of a compound comprising formula (I):

IT 282530-42-1P

DRWN

AΒ

LN.CNT 1846

(preparation of aminobenzoxazinones for the treatment of obesity)

IT 282530-42-1P

(preparation of aminobenzoxazinones for the treatment of obesity)

RN 282530-42-1 USPATFULL

CN 4H-3,1-Benzoxazin-4-one, 6-cyclopropyl-2-(phenylamino)- (9CI) (CA INDEX NAME)

L125 ANSWER 5 OF 10 USPATFULL on STN

AN 2003:188712 USPATFULL

TI Bicyclic androgen and progesterone receptor modulator compounds and

IN Zhi, Lin, San Diego, CA, UNITED STATES Tegley, Christopher, San Diego, CA, UNITED STATES

Pio, Barbara, San Diego, CA, UNITED STATES

Van Oerveren, Cornelis Arjan, San Diego, CA, UNITED STATES

Motamedi, Mehrnouch, San Diego, CA, UNITED STATES Martinborough, Esther, San Diego, CA, UNITED STATES

West, Sarah, San Diego, CA, UNITED STATES

Higuchi, Robert, Solana Beach, CA, UNITED STATES Hamann, Lawrence G., Cherry Hill, NJ, UNITED STATES

Farmer, Luc, Foxborough, MA, UNITED STATES

PΙ US 2003130505 A1 20030710

ΑI US 2002-299909 20021118 (10) A1

RLI Division of Ser. No. US 2000-649466, filed on 24 Aug 2000, PENDING

PRAI US 1999-150987P 19990827 (60)

DT Utility

FS APPLICATION

LREP Richard H. Pagliery, Brobeck, Phleger & Harrison LLP, 12390 El Camino Real, San Diego, CA, 92130-2081

CLMN Number of Claims: 41

ECL. Exemplary Claim: 1

No Drawings DRWN

LN.CNT 11834

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

The present invention is directed to compounds, pharmaceutical AB compositions, and methods for modulating processes mediated by AR and PR. More particularly, the invention relates to nonsteroidal compounds and compositions that are high affinity, high specificity agonists, partial agonists (i.e., partial activators and/or tissue-specific activators) and antagonists for AR and PR. Also provided are methods of making such compounds and pharmaceutical compositions, as well as critical intermediates used in their synthesis.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

328954-75-2P 328954-81-0P 328954-82-1P

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

IT 328954-75-2P

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

RN 328954-75-2 USPATFULL

CN2H-3,1-Benzoxazine-2-thione, 6-(1-cyclohexen-1-yl)-1,4-dihydro-4,4dimethyl- (9CI) (CA INDEX NAME)

L125 ANSWER 6 OF 10 USPATFULL on STN

ΑN 2003:137084 USPATFULL

Bicyclic androgen and progesterone receptor modulator compounds and TI methods

IN Zhi, Lin, San Diego, CA, United States Tegley, Christopher, San Diego, CA, United States Pio, Barbara, San Diego, CA, United States Van Oeveren, Cornelis Arjan, San Diego, CA, United States

Motamedi, Mehrnouch, San Diego, CA, United States Martinborough, Esther, San Diego, CA, United States.

West, Sarah, San Diego, CA, United States

PA Ligand Pharmaceuticals Incorporated, San Diego, CA, United States (U.S. corporation)

PΙ US 6566372 B1

US 2000-649466 20000824 (9) AΙ

<--PRAI US 1999-150987P 19990827 (60) <--

20030520

DT Utility FS GRANTED

EXNAM Primary Examiner: Dentz, Bernard

Paul, Hastings, Janofsky & Walker LLP

CLMN Number of Claims: 24 ECL Exemplary Claim: 1

0 Drawing Figure(s); 0 Drawing Page(s) DRWN

LN.CNT 10630

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

The present invention is directed to compounds, pharmaceutical compositions, and methods for modulating processes mediated by AR and PR. More particularly, the invention relates to nonsteroidal compounds and compositions that are high affinity, high specificity agonists, partial agonists (i.e., partial activators and/or tissue-specific activators) and antagonists for AR and PR. Also provided are methods of making such compounds and pharmaceutical compositions, as well as critical intermediates used in their synthesis.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

328954-75-2P 328954-81-0P 328954-82-1P

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

328954-75-2P

(preparation of quinolinones and related bicyclic compds. as androgen and progesterone receptor modulators)

RN 328954-75-2 USPATFULL

2H-3,1-Benzoxazine-2-thione, 6-(1-cyclohexen-1-yl)-1,4-dihydro-4,4dimethyl- (9CI) (CA INDEX NAME)

<--

L125 ANSWER 7 OF 10 USPATFULL on STN

2003:134622 USPATFULL

ΤI Cyclothiocarbamate derivatives as progesterone receptor modulators

IN Zhang, Puwen, Audubon, PA, UNITED STATES Fensome, Andrew, Wayne, PA, UNITED STATES Terefenko, Eugene A., Quakertown, PA, UNITED STATES Zhi, Lin, San Diego, CA, UNITED STATES Jones, Todd K., Solana Beach, CA, UNITED STATES

Edwards, James P., San Diego, CA, UNITED STATES

Tegley, Christopher M., Thousand Oaks, CA, UNITED STATES

Wrobel, Jay E., Lawrenceville, NJ, UNITED STATES Collins, Mark A., Norristown, PA, UNITED STATES

PΙ US 2003092711 A1 20030515

ΑI US 2002-140034 A1 20020506 (10)

RLI Continuation of Ser. No. US 2000-552354, filed on 19 Apr 2000, GRANTED, Pat. No. US 6436929

PRAI US 1999-183013P 19990504 (60)

DT Utility

FS APPLICATION

LREP HOWSON AND HOWSON, ONE SPRING HOUSE CORPORATION CENTER, BOX 457, 321 NORRISTOWN ROAD, SPRING HOUSE, PA, 19477

Number of Claims: 93 CLMN Exemplary Claim: 1 ECL

DRWN No Drawings

LN.CNT 4051

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

Methods of using compounds which are progesterone receptor agonists for AB contraception and the treatment of progesterone-related maladies alone or in combination with an estrogen receptor agonist or progesterone receptor antagonist are provided. These compounds have the structure: ##STR1##

wherein R.sub.1 and R.sub.2 are selected from the group of H, optionally substituted C.sub.1 to C.sub.6 alkyl, alkenyl, alkynyl, or alkynyl groups C.sub.3 to C.sub.8 cycloalkyl, aryl, substituted aryl, or heterocyclic groups, or COR.sup.A or NR.sup.BCOR.sup.A; or R.sup.1 and R.sup.2 are fused to form an optionally substituted ring structure as defined herein; R.sup.A and R.sup.B are as defined herein; R.sup.3 is H, OH, NH.sub.2, COR.sup.C, or optionally substituted C.sub.1 to C.sub.6 alkyl, C.sub.3 to C.sub.6 alkenyl, or alkynyl groups; R.sup.C is as defined herein; Q.sup.1 is S, NR.sup.7, or CR.sup.8R.sup.9; R.sup.5 is an optionally trisubstituted benzene ring or an optionally substituted five or six membered heterocyclic ring.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

304853-32-5P 304853-33-6P 304853-35-8P

304853-37-0P 304853-38-1P 304853-39-2P

304853-40-5P 304853-41-6P 304853-42-7P

304853-43-8P 304853-44-9P 304853-45-0P

304853-46-1P 304853-47-2P 304853-48-3P

304853-49-4P 304853-50-7P 304853-51-8P 304853-52-9P 304853-53-0P 304853-54-1P 304853-55-2P 304853-56-3P 304853-57-4P 304853-58-5P 304853-59-6P 304853-60-9P 304853-61-0P 304853-62-1P 304853-63-2P 304853-64-3P 304853-65-4P 304853-66-5P 304853-70-1P 304853-71-2P 304853-72-3P 304853-73-4P 304853-74-5P 304853-75-6P 304853-76-7P 304853-77-8P 304853-78-9P 304853-79-0P 304853-82-5P 304853-83-6P 304853-81-4P 304853-85-8P 304853-86-9P 304853-87-0P 304853-88-1P

(preparation of cyclothiocarbamate derivs. as progesterone receptor modulators)

IT 304853-95-0P

(preparation of cyclothiocarbamate derivs. as progesterone receptor modulators)

IT 304853-32-5P

(preparation of cyclothiocarbamate derivs. as progesterone receptor modulators)

RN 304853-32-5 USPATFULL

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

L125 ANSWER 8 OF 10 USPATFULL on STN

AN 2003:38174 USPATFULL

TI 2-Oxy-benzoxazinone derivatives for the treatment of obesity

IN Hodson, Harold Francis, Beckenham, UNITED KINGDOM

Downham, Robert, Cambridge, UNITED KINGDOM

Mitchell, Timothy John, Cambridge, UNITED KINGDOM

Carr, Beverley Jane, Royston, UNITED KINGDOM

Dunk, Christopher Robert, Ely, UNITED KINGDOM

Palmer, Richard Michael John, Kent, UNITED KINGDOM

PI US 2003027821 A1 20030206

US 6624161 B2 20030923

AI US 2001-901887 A1 20010706 (9) <--

RLI Continuation of Ser. No. WO 2000-GB32, filed on 6 Jan 2000, UNKNOWN

PRAI GB 1999-413 19990108 <--

GB 1999-17294 19990722 <--

DT Utility

FS APPLICATION

LREP Choate, Hall & Stewart, Exchange Place, 53 State Street, Boston, MA,

CLMN Number of Claims: 53

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 1822

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The use of a compound comprising formula (I): ##STR1##

(I)

or a salt, ester, amide or prodrug therof in the inhibition of an enzyme whose preferred mode of action is to catalyse the hydrolysis of an ester functionality, e.g. in the control and inhibition of unwanted enzymes in products and processes. The compounds are also useful in medicine e.g. in the treatment of obesity and related conditions. The invention also relates to novel compounds within formula (I), to processes for preparing them and pharmaceutical compositions containing them.

In formula (I) A is a 6-membered aromatic or heteroaromatic ring; and R.sup.1 is a branched or unbranched alkyl (optionally interrupted by one or more oxygen atoms), alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl, arylalkyl, reduced arylalkyl, arylalkenyl, heteroaryl, heteroarylalkyl, heteroarylalkenyl, reduced aryl, reduced heteroaryl, reduced heteroarylalkyl or a substituted derivative of any of the foregoing groups.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 282530-42-1P

(preparation of aminobenzoxazinones for the treatment of obesity)

IT 282530-42-1P

(preparation of aminobenzoxazinones for the treatment of obesity)

RN 282530-42-1 USPATFULL

CN 4H-3,1-Benzoxazin-4-one, 6-cyclopropyl-2-(phenylamino)- (9CI) (CA INDEX NAME)

L125 ANSWER 9 OF 10 USPATFULL on STN

AN 2002:209520 USPATFULL

TI Cyclothiocarbamate derivatives as progesterone receptor modulators

IN Zhang, Puwen, Audubon, PA, United States Fensome, Andrew, Wayne, PA, United States

Terefenko, Eugene A., Quakertown, PA, United States

Zhi, Lin, San Diego, CA, United States

Jones, Todd K., Solana Beach, CA, United States Edwards, James P., San Diego, CA, United States

Tegley, Christopher M., Thousand Oaks, CA, United States

Wrobel, Jay E., Lawrenceville, NJ, United States Collins, Mark A., Norristown, PA, United States

PA Wyeth, Madison, NJ, United States (U.S. corporation)

Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S.

corporation)

PI US 6436929 B1 20020820 <-AI US 2000-552354 20000419 (9) <-PRAI US 1999-183013P 19990504 (60) <--

DT Utility

FS GRANTED

EXNAM Primary Examiner: Raymond, Richard L.; Assistant Examiner: Truong,

Tamthom N.

LREP Howson and Howson
CLMN Number of Claims: 111
ECL Exemplary Claim: 1

DRWN 0 Drawing Figure(s); 0 Drawing Page(s)

LN.CNT 3617

IT 304853-32-5P

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides compounds which are agonists of the progesterone receptor and have the structures: ##STR1##

wherein R.sub.1 and R.sub.2 are independent substituents selected from the group of H, optionally substituted C.sub.1 to C.sub.6 alkyl, alkenyl, alkynyl, or alkynyl groups C.sub.3 to C.sub.8 cycloalkyl, aryl, substituted aryl, or heterocyclic groups, or COR.sup.A or NR.sup.BCOR.sup.A; or R.sup.1 and R.sup.2 are fused to form an optionally substituted 3 to 8 membered Spiro cyclic alkyl or alkenyl ring or a Spiro cyclic ring containing one to three heteroatoms selected from O, S and N; R.sup.A is selected from H, amino, or optionally substituted C.sub.1 to C.sub.3 alkyl, aryl, C.sub.1 to C.sub.3 alkoxy, or C.sub.1 to C.sub.3 aminoalkyl groups; R.sup.B is H, C.sub.1 to C.sub.3 alkyl, or substituted C.sub.1 to C.sub.3 alkyl; R.sup.3 is H, OH, NH.sub.2, COR.sup.C, or optionally substituted C.sub.1 to C.sub.6 alkyl, C.sub.3 to C.sub.6 alkenyl, or alkynyl groups, R.sup.C is selected from H or optionally substituted C.sub.1 to C.sub.3 alkyl, aryl, C.sub.1 to C.sub.3 alkoxy, or C.sub.1 to C.sub.3 aminoalkyl groups; Q.sup.1 is S, NR.sup.7, or CR.sup.8R.sup.9; R.sup.5 is an optionally trisubstituted benzene ring or an optionally substituted five or six membered heterocyclic ring with 1, 2, or 3 ring heteroatoms selected from the group of O, S, SO, SO.sub.2 or NR.sup.6; or a pharmaceutically acceptable salt thereof, as well as methods of using these compounds for contraception and the treatment of progesterone-related maladies.

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CAS INDEXING IS AVAILABLE FOR THIS PATENT.
     304853-32-5P 304853-33-6P 304853-35-8P
      304853-37-0P 304853-38-1P 304853-39-2P
      304853-40-5P 304853-41-6P 304853-42-7P
      304853-43-8P 304853-44-9P 304853-45-0P
      304853-46-1P 304853-47-2P 304853-48-3P
      304853-49-4P 304853-50-7P 304853-51-8P
      304853-52-9P 304853-53-0P 304853-54-1P
      304853-55-2P 304853-56-3P 304853-57-4P
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      304853-67-6P 304853-68-7P 304853-69-8P
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      304853-76-7P 304853-77-8P 304853-78-9P
      304853-79-0P 304853-80-3P 304853-81-4P
      304853-82-5P 304853-83-6P 304853-84-7P
      304853-85-8P 304853-86-9P 304853-87-0P
      304853-88-1P
        (preparation of cyclothiocarbamate derivs. as progesterone receptor
        modulators)
TΤ
     304853-95-0P
        (preparation of cyclothiocarbamate derivs. as progesterone receptor
        modulators)
```

(preparation of cyclothiocarbamate derivs. as progesterone receptor

```
modulators)
```

RN 304853-32-5 USPATFULL

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

```
L125 ANSWER 10 OF 10 USPATFULL on STN
AN
       92:103164 USPATFULL
ΤI
       Imidazole substituted benzoxazine or benzothiazine derivatives
IN
       Kim, Moohi Y., Seoul, Korea, Republic of
       Shin, Hyun T., Seoul, Korea, Republic of
       Lee, Choon W., Seoul, Korea, Republic of
       Kim, Joon W., Kyungki, Korea, Republic of
       Kim, Soon H., Kyungki, Korea, Republic of
       Choi, Youngmoon, Seoul, Korea, Republic of
       Son, Moon H., Kyungki, Korea, Republic of
PA
       Dong-A Pharm. Co., Ltd., Seoul, Korea, Republic of (non-U.S.
       corporation)
PΙ
       US 5171851
                               19921215
AΤ
       US 1991-674183
                               19910325 (7)
                                                                     <--
PRAI
       KR 1990-3989
                           19900324
DT
       Utility
FS
       Granted
       Primary Examiner: Shah, Mukund J.; Assistant Examiner: Dalton, Philip I.
EXNAM
       Birch, Stewart, Kolasch & Birch
       Number of Claims: 26
CLMN
ECL
       Exemplary Claim: 1
       No Drawings
DRWN
LN.CNT 813
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
       A benzoxazine or benzothiazine derivative of the formula (A), ##STR1##
       wherein R.sub.1, R.sub.2 and R.sub.3 are the same or different and
       represent a hydrogen atom or a C.sub.1-4 alkyl group; or R.sub.1 and
       R.sub.2 can be joined together along with the imidazole ring to form a
       benzimidazole; X and Y are the same or different and represent an oxygen
       or sulfur atom; or a pharmaceutically acceptable salt thereof, exhibits
       an excellent inotropic effect and can be used as a cardiac stimulant.
```

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 145622-92-0P

(preparation of, as pos. inotropic)

IT 145622-92-0P

(preparation of, as pos. inotropic)

RN 145622-92-0 USPATFULL

CN 2H-3,1-Benzoxazine-2-thione, 1,4-dihydro-8-methyl-6-(4-methyl-1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)

=> fil reg FILE 'REGISTRY' ENTERED AT 07:57:47 ON 05 JUL 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 JUL 2005 HIGHEST RN 853727-85-2 DICTIONARY FILE UPDATES: 4 JUL 2005 HIGHEST RN 853727-85-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> s 123 not 1115 L127 76 L23 NOT L115

=> d ide can tot

L127 ANSWER 1 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN
RN 639085-00-0 REGISTRY
ED Entered STN: 19 Jan 2004
CN 1,3-Benzenedicarbonitrile, 5-(1,4-dihydro-1-mercapto-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 5-(4,4-Dimethyl-1,2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)isophthalonitrile

3D CONCORD FS

MF C18 H13 N3 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

L127 ANSWER 2 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-48-7 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-[1,4-dihydro-2-thioxo-4,4bis(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

1-Methyl-5-[2-thioxo-4,4-bis(trifluoromethyl)-1,4-dihydro-2H-3,1-CN benzoxazin-6-yl]-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C16 H9 F6 N3 O S

SR CA

STN Files: CA, CAPLUS, TOXCENTER, USPATFULL LC

$$\begin{array}{c|c} Me & H & S \\ \hline \\ NC & N & O \\ \hline \\ F_3C & CF_3 \\ \end{array}$$

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L127 ANSWER 3 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

638989-46-5 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclopentan]-6-yl]-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C18 H17 N3 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L127 ANSWER 4 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-44-3 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

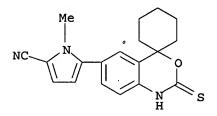
CN 1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C19 H19 N3 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

jan delaval - 5 july 2005

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L127 ANSWER 5 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-41-0 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(4-ethyl-1,4-dihydro-4-methyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4-Ethyl-4-methyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C17 H17 N3 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L127 ANSWER 6 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-38-5 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(4,4-diethyl-1,4-dihydro-2-thioxo-2H-3,1-benzoxazin-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Diethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C18 H19 N3 O S

SR CA

$$\begin{array}{c|c} Me & H \\ N & N \\ \end{array}$$

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L127 ANSWER 7 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-33-0 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-Methyl-5-[2-thioxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclobutan]-6-yl]-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C17 H15 N3 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L127 ANSWER 8 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560992-05-4 REGISTRY

ED Entered STN: 05 Aug 2003

CN Benzonitrile, 4-(8-bromo-1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-2-fluoro-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H12 Br F N2 O S

SR CA

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 9 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560992-04-3 REGISTRY

ED Entered STN: 05 Aug 2003

CN 2H-3,1-Benzoxazine-2-thione, 8-bromo-6-(4-chloro-3-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H12 Br Cl F N O S

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 10 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560992-03-2 REGISTRY

ED Entered STN: 05 Aug 2003

CN Benzonitrile, 3-(1-ethyl-1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H17 F N2 O S

SR CA

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 11 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560992-02-1 REGISTRY

ED Entered STN: 05 Aug 2003

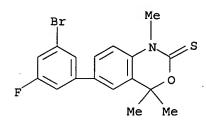
CN 2H-3,1-Benzoxazine-2-thione, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-1,4,4-trimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H15 Br F N O S

SR CA

LC STN Files: CA, CAPLUS



# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 12 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560992-01-0 REGISTRY

ED Entered STN: 05 Aug 2003

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-bromophenyl)-1,4-dihydro-1,4,4-trimethyl-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H16 Br N O S

SR CA

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 13 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560992-00-9 REGISTRY

ED Entered STN: 05 Aug 2003

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4,4-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C28 H22 Cl N O S

SR CA

LC STN Files: CA, CAPLUS

C1
$$\begin{array}{c} H \\ N \\ S \\ \end{array}$$

$$\begin{array}{c} S \\ O \\ Ph-CH_2 \\ CH_2-Ph \\ \end{array}$$

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 14 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560991-99-3 REGISTRY

ED Entered STN: 05 Aug 2003

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-5-(trifluoromethoxy)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H13 F3 N2 O2 S

SR CA

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 15 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 560991-98-2 REGISTRY

ED Entered STN: 05 Aug 2003

CN Benzonitrile, 3-bromo-5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H13 Br N2 O S

SR CA

LC STN Files: CA, CAPLUS

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:111065

L127 ANSWER 16 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 328954-82-1 REGISTRY

ED Entered STN: 26 Mar 2001

CN 2H-3,1-Benzoxazine-2-thione, 1,4-dihydro-6-(3-hydroxy-1-cyclohexen-1-yl)-4,4-dimethyl-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H19 N O2 S

SR . CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:207727

L127 ANSWER 17 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 328954-81-0 REGISTRY

ED Entered STN: 26 Mar 2001

CN 2-Cyclohexen-1-one, 3-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H17 N O2 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

. 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:207727

L127 ANSWER 18 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 328954-75-2 REGISTRY

ED Entered STN: 26 Mar 2001

CN 2H-3,1-Benzoxazine-2-thione, 6-(1-cyclohexen-1-yl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H19 N O S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:207727

L127 ANSWER 19 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-95-0 REGISTRY

ED Entered STN: 29 Nov 2000

CN 1H-Pyrrole-1-carboxylic acid, 2-cyano-5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:

CN 2-Cyano-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-pyrrole-1-carboxylic acid tert-Butyl ester

FS 3D CONCORD

MF C20 H21 N3 O3 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 20 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-88-1 REGISTRY

ED Entered STN: 29 Nov 2000

CN 3-Thiophenecarbonitrile, 2-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)thiophene-3-

carbonitrile

FS 3D CONCORD

MF C15 H12 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 21 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-87-0 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-bromophenyl)-1,4-dihydro-4,4-dimethyl-

(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Bromophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H14 Br N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 22 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-86-9 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 4-butyl-5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-Butyl-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)thiophene-2-carbonitrile

FS 3D CONCORD

MF C19 H20 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} & H \\ N \\ \hline \\ NC \\ \hline \\ SU-n \\ \end{array}$$

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 23 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-85-8 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Furancarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-

benzoxazin-6-yl) - (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-2-furonitrile

FS 3D CONCORD

MF C15 H12 N2 O2 S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 24 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-84-7 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-4-propyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-4propylthiophene-2-carbonitrile

FS 3D CONCORD

MF C18 H18 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} & H \\ N \\ \hline \\ NC \\ N$$

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 25 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-83-6 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chloro-4-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Chloro-4-fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H13 Cl F N O S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 26 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-82-5 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 5-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-

4,1'-cyclohexan]-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-2-

thiophenecarbonitrile

FS 3D CONCORD

MF C18 H16 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 27 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-81-4 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 5-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl)-4-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-4-methyl-2-thiophenecarbonitrile

FS 3D CONCORD

MF C19 H18 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 28 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-80-3 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'cyclohexan]-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]benzonitrile

FS 3D CONCORD

MF C20 H18 N2 O S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 29 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-79-0 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-fluoro-5-(8-fluoro-1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-Fluoro-5-(8-fluoro-4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)benzonitrile

FS 3D CONCORD

MF C17 H12 F2 N2 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 30 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-78-9 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)thiophene-2-carbonitrile

FS 3D CONCORD

MF C15 H12 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 31 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-77-8 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-bromo-5-fluorophenyl)-1,4-dihydro-4,4-

dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Bromo-5-fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H13 Br F N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 32 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-76-7 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-Benzyl-6-(3-chlorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C22 H18 Cl N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$C1$$
 $ph-CH_2$  Me

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 33 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-75-6 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(2-chlorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(2-Chlorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H14 Cl N O S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 34 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-74-5 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 1,4-dihydro-6-(3-methoxyphenyl)-4,4-dimethyl-

(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Methoxyphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C17 H17 N O2 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 35 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

jan delaval - 5 july 2005

RN 304853-73-4 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-4,4-diethyl-1,4-dihydro-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Chlorophenyl)-4,4-diethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C18 H18 Cl N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 36 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-72-3 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 1,4-dihydro-4,4-dimethyl-6-(3-nitrophenyl)-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4,4-Dimethyl-6-(3-nitrophenyl)-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H14 N2 O3 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 4 REFERENCES IN FILE CA (1907 TO DATE)
- 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

jan delaval - 5 july 2005

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 37 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-71-2 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-(8-bromo-1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-(8-Bromo-4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-5-fluorobenzonitrile

FS 3D CONCORD

MF C17 H12 Br F N2 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 38 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-70-1 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(2,3-difluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(2,3-Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H13 F2 N O S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 39 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-69-8 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-

4-fluoro- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-4-fluorobenzonitrile

FS 3D CONCORD

MF C17 H13 F N2 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 40 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN RN 304853-68-7 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(4-fluorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(4-Fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H14 F N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 41 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-67-6 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3,4-difluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3,4-Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H13 F2 N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} F & H & S \\ \hline & N & S \\ \hline & Me & Me \end{array}$$

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 4 REFERENCES IN FILE CA (1907 TO DATE)
- 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 42 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-66-5 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(2-fluorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(2-Fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H14 F N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 43 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-65-4 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-[3-fluoro-5-(trifluoromethyl)phenyl]-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-[3-Fluoro-5-(trifluoromethyl)phenyl]-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C17 H13 F4 N O S

SR CA

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 139:111065

REFERENCE 3: 133:350228

L127 ANSWER 44 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-64-3 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-fluorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H14 F N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 45 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-63-2 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-5-methoxy- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-5-methoxybenzonitrile

FS 3D CONCORD

MF C18 H16 N2 O2 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 46 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-62-1 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-fluoro-5-methoxyphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Fluoro-5-methoxyphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C17 H16 F N O2 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 47 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-61-0 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3,5-difluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3,5-Difluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H13 F2 N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 48 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-60-9 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-chloro-5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-Chloro-5-(4,4-dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6yl)benzonitrile

FS 3D CONCORD

MF C17 H13 Cl N2 O S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 49 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-59-6 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-(2-propenyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-Allyl-6-(3-chlorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

CHIOHE

FS 3D CONCORD

MF  $\cdot$  C18 H16 Cl N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$C1$$
 $H_2C = CH - CH_2$ 
 $Me$ 

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 50 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-58-5 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4-methyl-4-phenyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Chlorophenyl)-4-methyl-4-phenyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C21 H16 Cl N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 51 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-57-4 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 4,4-diethyl-1,4-dihydro-6-(3-nitrophenyl)(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4,4-Diethyl-6-(3-nitrophenyl)-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C18 H18 N2 O3 S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 52 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-56-3 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Furancarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-2-furonitrile

FS 3D CONCORD

MF C15 H12 N2 O2 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 53 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN.

RN 304853-55-2 REGISTRY

ED Entered STN: 29 Nov 2000

CN 1,3-Benzenedicarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H13 N3 O S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:53469

REFERENCE 2: 139:111065

REFERENCE 3: 133:350228

L127 ANSWER 54 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-54-1 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3,5-dichlorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3,5-Dichlorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H13 Cl2 N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 55 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN RN 304853-53-0 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-5-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-5-CN methylbenzonitrile

FS 3D CONCORD

C18 H16 N2 O S MF

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 56 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-52-9 REGISTRY

ED Entered STN: 29 Nov 2000

CNBenzonitrile, 3-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-

cyclohexan]-6-yl)-5-fluoro- (9CI) (CA INDEX NAME)

OTHER NAMES:

3-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-5-CN fluorobenzonitrile

FS 3D CONCORD

MF C20 H17 F N2 O S

SR CA

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 57 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-51-8 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-[3-bromo-5-(trifluoromethoxy)phenyl]-1,4dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Bromo-5-trifluoromethoxyphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1benzoxazine-2-thione

FS 3D CONCORD

MF C17 H13 Br F3 N O2 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 58 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-50-7 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-bromo-5-methylphenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Bromo-5-methylphenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2thione

FS 3D CONCORD

MF C17 H16 Br N O S

SR CA

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 59 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-49-4 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chloro-5-fluorophenyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Chloro-5-fluorophenyl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C16 H13 Cl F N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} C1 & H \\ N & S \\ \hline \\ Me & Me \\ \end{array}$$

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 60 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-48-3 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(5-bromo-3-pyridinyl)-1,4-dihydro-4,4-dimethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(5-Bromopyridin-3-yl)-4,4-dimethyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C15 H13 Br N2 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 61 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-47-2 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-2-fluoro-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-2fluorobenzonitrile

FS 3D CONCORD

MF C17 H13 F N2 O S

SR CA

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER '62 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-46-1 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 4-(1,2-dihydro-2-thioxospiro[4H-3,1-benzoxazine-

4,1'-cyclohexan]-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[1,2-Dihydro-2-thioxospiro[4H-3,1-benzoxazin-4,1'-cyclohexan]-6-yl]-2-

thiophenecarbonitrile

FS 3D CONCORD

MF C18 H16 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 63 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-45-0 REGISTRY

ED Entered STN: 29 Nov 2000

CN 1H-Pyrrole-2-carbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-1-ethyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-ethyl-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C17 H17 N3 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} Et & H \\ NC & N \\ \hline \end{array}$$

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 64 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-44-9 REGISTRY

ED Entered STN: 29 Nov 2000

CN 3-Thiophenecarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)thiophene-3-carbonitrile

FS 3D CONCORD

MF C15 H12 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

jan delaval - 5 july 2005

### 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 65 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-43-8 REGISTRY

ED Entered STN: 29 Nov 2000

CN 1H-Pyrrole-2-carbothioamide, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-pyrrole-2-carbothioamide

FS 3D CONCORD

MF C15 H15 N3 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} S & H & H \\ H_2N-C & N & Me & Me \end{array}$$

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 66 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-41-6 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Pyridineacetonitrile, 6-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN [6-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)pyridin-2-yl]acetonitrile

FS 3D CONCORD

MF C17 H15 N3 O S

SR CA

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 67 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-40-5 REGISTRY

ED Entered STN: 29 Nov 2000

CN 1H-Pyrrole-2-carbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C15 H13 N3 O S

SR . CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} H & H \\ N & O \\ \hline \\ Me & Me \\ \end{array}$$

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 68 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-39-2 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 5-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-

benzoxazin-6-yl)-4-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-4-methylthiophene-2-carbonitrile

FS 3D CONCORD

MF C16 H14 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 133:350228

L127 ANSWER 69 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-38-1 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-fluorophenyl)-1,4-dihydro-4-methyl-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Fluorophenyl)-4-methyl-1,4-dihydro-2H-3,1-benzoxazine-2-thione

FS 3D CONCORD

MF C15 H12 F N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 70 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-37-0 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6yl)benzonitrile

FS 3D CONCORD

MF C17 H14 N2 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 71 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-35-8 REGISTRY

ED Entered STN: 29 Nov 2000

CN Benzonitrile, 3-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-benzoxazin-6-yl)-5-fluoro-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)-5-fluorobenzonitrile

FS 3D CONCORD

MF C17 H13 F N2 O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 72 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-33-6 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2-Thiophenecarbonitrile, 4-(1,4-dihydro-4,4-dimethyl-2-thioxo-2H-3,1-

benzoxazin-6-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-(4,4-Dimethyl-2-thioxo-1,4-dihydro-2H-benzo[d][1,3]oxazin-6-yl)thiophene-2-carbonitrile

FS 3D CONCORD

MF C15 H12 N2 O S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c|c} & H & S \\ \hline NC & & \\ S & & \\ \hline Me & Me \end{array}$$

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 139:111065

REFERENCE 3: 133:350228

L127 ANSWER 73 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304853-32-5 REGISTRY

ED Entered STN: 29 Nov 2000

CN 2H-3,1-Benzoxazine-2-thione, 6-(3-chlorophenyl)-1,4-dihydro-4,4-dimethyl-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-(3-Chlorophenyl)-4,4-dimethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-thione

FS 3D CONCORD

MF C16 H14 Cl N O S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 139:111065

REFERENCE 4: 133:350228

L127 ANSWER 74 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 282530-42-1 REGISTRY

ED Entered STN: 02 Aug 2000

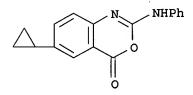
CN 4H-3,1-Benzoxazin-4-one, 6-cyclopropyl-2-(phenylamino)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H14 N2 O2

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:105042

L127 ANSWER 75 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 145622-92-0 REGISTRY

ED Entered STN: 29 Jan 1993

CN 2H-3,1-Benzoxazine-2-thione, 1,4-dihydro-8-methyl-6-(4-methyl-1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H13 N3 O S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

$$\stackrel{\mathsf{Me}}{\underset{\mathsf{N}}{\longrightarrow}} \stackrel{\mathsf{H}}{\underset{\mathsf{N}}{\longrightarrow}} \mathsf{S}$$

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 118:213099

REFERENCE 2: 118:101972

L127 ANSWER 76 OF 76 REGISTRY COPYRIGHT 2005 ACS on STN

RN 119198-26-4 REGISTRY

ED Entered STN: 24 Feb 1989

CN Piperazine, 1-(1,4-dihydro-2-thioxo-2H-3,1-benzoxazin-6-yl)-4-(3,4-

dimethoxybenzoyl) - (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-3,1-Benzoxazine, piperazine deriv.

FS 3D CONCORD

MF C21 H23 N3 O4 S

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT

(\*File contains numerically searchable property data)

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## 1 REFERENCES IN FILE CA (1907 TO DATE)

jan delaval - 5 july 2005

## 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 110:95163

#### => d ide can tot 122

L22 ANSWER 1 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-51-2 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-[1,4-dihydro-2-oxo-4,4-bis(trifluoromethyl)-2H-3,1-benzoxazin-6-yl]-1-methyl- (9CI) (CA INDEX NAME)

#### OTHER NAMES:

CN 1-Methyl-5-[2-oxo-4,4-bis(trifluoromethyl)-1,4-dihydro-2H-3,1-benzoxazin-6yl]-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C16 H9 F6 N3 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 2 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-50-1 REGISTRY

ED Entered STN: 19 Jan 2004

CN 2H-3,1-Benzoxazin-2-one, 6-bromo-1,4-dihydro-4,4-bis(trifluoromethyl)-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-Bromo-4,4-bis(trifluoromethyl)-1,4-dihydro-2H-3,1-benzoxazin-2-one

FS 3D CONCORD

MF C10 H4 Br F6 N O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 3 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-49-8 REGISTRY

ED Entered STN: 19 Jan 2004

CN 2H-3,1-Benzoxazin-2-one, 1,4-dihydro-4,4-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4,4-Bis(trifluoromethyl)-1,4-dihydro-2H-3,1-benzoxazin-2-one

FS 3D CONCORD

MF C10 H5 F6 N O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 4 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-47-6 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-

4,1'-cyclopentan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-Methyl-5-[2-oxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclopentan]-6-yl]-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C18 H17 N3 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 5 OF 14 REGISTRY COPYRIGHT 2005 ACS ON STN

RN 638989-45-4 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-

4,1'-cyclohexan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-Methyl-5-[2-oxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclohexan]-6-yl]-

1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C19 H19 N3 O2

SR CA

LC STN Files: CA, CAPLUS, PROUSDDR, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 6 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

jan delaval - 5 july 2005

RN 638989-43-2 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(4-ethyl-1,4-dihydro-4-methyl-2-oxo-2H-3,1-benzoxazin-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4-Ethyl-4-methyl-2-oxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C17 H17 N3 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 7 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-42-1 REGISTRY

ED Entered STN: 19 Jan 2004

CN 2H-3,1-Benzoxazin-2-one, 6-bromo-4-ethyl-1,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-Bromo-4-ethyl-4-methyl-1,4-dihydro-2H-3,1-benzoxazin-2-one

FS 3D CONCORD

MF C11 H12 Br N O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 8 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-40-9 REGISTRY

ED Entered STN: 19 Jan 2004

CN 2H-3,1-Benzoxazin-2-one, 6-bromo-4,4-diethyl-1,4-dihydro- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-Bromo-4,4-diethyl-1,4-dihydrobenzo[d][1,3]oxazin-2-one

FS 3D CONCORD

MF C12 H14 Br N O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 9 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-39-6 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(4,4-diethyl-1,4-dihydro-2-oxo-2H-3,1-

benzoxazin-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-(4,4-Diethyl-2-oxo-1,4-dihydro-2H-3,1-benzoxazin-6-yl)-1-methyl-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C18 H19 N3 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 10 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-37-4 REGISTRY

ED Entered STN: 19 Jan 2004

CN 1H-Pyrrole-2-carbonitrile, 5-(1,2-dihydro-2-oxospiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-6-yl)-1-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-Methyl-5-[2-oxo-1,2-dihydrospiro[3,1-benzoxazine-4,1'-cyclobutan]-6-yl]-1H-pyrrole-2-carbonitrile

FS 3D CONCORD

MF C17 H15 N3 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 11 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-36-3 REGISTRY

ED Entered STN: 19 Jan 2004

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one, 6-bromo- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-Bromospiro[3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one

FS 3D CONCORD

MF C11 H10 Br N O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 12 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 638989-35-2 REGISTRY

ED Entered STN: 19 Jan 2004

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Spiro[3,1-benzoxazine-4,1'-cyclobutan]-2(1H)-one

FS 3D CONCORD

MF C11 H11 N O2

SR CA

LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

L22 ANSWER 13 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 305799-84-2 REGISTRY

ED Entered STN: 01 Dec 2000

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-one, 6-bromo- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 6-Bromospiro[4H-3,1-benzoxazine-4,1'-cyclopentan]-2(1H)-one

FS 3D CONCORD

MF C12 H12 Br N O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

REFERENCE 2: 140:53469

REFERENCE 3: 137:201317

REFERENCE 4: 133:350229

REFERENCE 5: 133:350205

L22 ANSWER 14 OF 14 REGISTRY COPYRIGHT 2005 ACS on STN

RN 304854-04-4 REGISTRY

ED Entered STN: 29 Nov 2000

CN Spiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one, 6-bromo- (9CI) (CA

INDEX NAME)

OTHER NAMES:
CN 6-Bromospiro[4H-3,1-benzoxazine-4,1'-cyclohexan]-2(1H)-one

FS 3D CONCORD

MF C13 H14 Br N O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT7, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:71530

```
REFERENCE
            2: 140:53469
REFERENCE
                137:201317
            3:
REFERENCE
               133:350229
            4:
REFERENCE
            5:
                133:350228
REFERENCE
            6: 133:350205
=> d his
     (FILE 'HOME' ENTERED AT 07:18:36 ON 05 JUL 2005)
                SET COST OFF
     FILE 'REGISTRY' ENTERED AT 07:18:43 ON 05 JUL 2005
L1
                STR
              5 S L1
L2
     FILE 'HCAPLUS' ENTERED AT 07:20:57 ON 05 JUL 2005
L3
              1 S US20040014798/PN OR (US2003-601968# OR WO2003-US19860 OR US20
                E FONSOME A/AU
                E FENSOME A/AU
L4
             37 S E3, E6, E7
                E HARRISON D/AU
L5
            123 S E3, E8, E114-E116, E118
                E WINNEKER R/AU
L6
             59 S E4-E7
                E ZHANG P/AU
L7
            307 S E3,E17
                E ZHANG PU/AU
L8
            136 S E3, E24, E25
                E ZHANG P/AU
L9
            694 S E3-E20.
                E KERN J/AU
L10
            203 S E3, E5, E29-E31, E34
                E TEREFENKO E/AU
L11
             24 S E4-E7
                E WYETH/PA, CS
                E WYET/PA,CS
L12
           4429 S E4-E7 OR WYETH?/PA,CS
                SEL RN L3
     FILE 'REGISTRY' ENTERED AT 07:24:43 ON 05 JUL 2005
L13
             84 S E1-E84
L14
                STR L1
L15
             50 S L14
L16
           1063 S L14 FUL
                SAV L16 KWON601/A
L17
             60 S L13 AND L16
L18
             24 S L13 NOT L17
L19
             10 S L18 AND NR>=3 NOT C5-C6-C6-C6/ES
L20
             14 S L18 NOT L19
L21
             4 S L20 AND NCOC3-C6/ES
L22
             14 S L19, L21
L23
             77 S L1 FUL SUB=L16
                SAV L23 KWON601A/A
L24
             17 S L23 NOT L17
```

```
FILE 'HCAOLD' ENTERED AT 07:28:34 ON 05 JUL 2005
L25
               0 S L23
L26
               0 S L22
     FILE 'HCAPLUS' ENTERED AT 07:28:44 ON 05 JUL 2005
L27
              10 S L23
L28
              6 S L22
L29
              13 S L27, L28
L30
               6 S L29 AND L3-L12
                 E HIRSUTISM/CT
                 E E3+ALL
L31
             968 S E4
L32
           1517 S E4,E5/BI
                 E HYPERTRICH
L33
            134 S E4-E7
                 E HIRSUT
L34
               1 S L29 AND L31-L33
             1 S L29 AND HIRSUT?
L35
                 E ACNE/CT
L36
           3716 S E3-E8
                 E E3+ALL
           3741 S E6+NT
L37
L38
           6082 S E6, E7/BI
L39
            243 S PIMPL?
L40
           6272 S ACNE?
                 E ACNE/CT
                 E E6+ALL
L41
          301 S E2
L42
               1 S L29 AND L36-L41
                 E ECZEMA/CT
L43
           2222 S E3,E4
                 E E3+ALL
L44
           2222 S E9
           3655 S E9,E10/BI
L45
L46
               1 S L29 AND ECZEM?
               1 S L3, L34, L35, L42, L46
L47
                 E SKIN/CT
                 E E3+ALL
L48
         105580 S E6+OLD, NT
L49
         124391 S E6+PFT, RT
                 E E37+ALL
L50
         139455 S E5+OLD, NT, PFT, RT
                 E E181+ALL
         155162 S E3+OLD, NT, PFT, RT
1.51
         142584 S E13+OLD, NT, PFT, RT
L52
L53
          16036 S E16+OLD, NT, PFT, RT
               2 S L29 AND L48-L53
L54
                 E HAIR/CT
          52596 S E3+OLD, NT, PFT, RT
L55
L56
          52664 S E43+OLD, NT, PFT, RT
L57
          20289 S E86+OLD, NT, PFT, RT
                 E SKIN CONDITION/CT
                 E E4+ALL
L58
           1145 S E2
L59
               1 S L29 AND L55-L58
L60
               2 S L47, L54, L59
               4 S L29 AND PROGESTERONE (L) RECEPTOR (L) ?MODULAT?
L61
                 E PROGESTERONE RECEPTOR/CT
L62
           3809 S E8-E14
                 E E8+ALL
```

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L63
             4894 S E11+OLD, NT
 L64
             9236 S E11+PFT,RT
 L65
                7 S L29 AND L62-L64
                  E ENDOMETRIOSIS/CT
                  E E3+ALL
 L66
             1849 S E2
 L67
             2470 S E1/BI
                  E BENIGN PROSTATIC HYPERTROPHY/CT
                  E E3+ALL
 L68
             1469 S E3
 L69
              655 S E1/BI
                  E BENIGN PROSTATIC HYPERTROPHY/CT
 L70
             2319 S E2/BI
                  E ENDOMETRIUM/CT
                  E E3+ALL
 L71
             9801 S E2
 L72
              647 S E6, E7
 L73
             1424 S E9, E10
 L74
              854 S E12, E13
 L75
              370 S E15, E16
 L76
              386 S E18, E19
 L77
              243 S E21, E22
 L78
            3398 S E24
                  E OVARY/CT
 L79
           57237 S E3+OLD, NT
 L80
            18487 S E54+OLD, NT
 L81
            14597 S E67+OLD, NT
                  E BREAST/CT
                  E E3+ALL
                  E E2+ALL
 L82
           63582 S E3+OLD, NT
 L83
           50658 S E9+OLD, NT
                  E MAMMARY GLAND/CT
 L84
           65709 S E3+OLD, NT OR E47+OLD, NT
 L85
           47677 S E53+OLD, NT
                  E COLON/CT
                  E E3+ALL
 L86
           31294 S E1,E2
                  E COLON, DISEASE/CT
                  E E2+ALL
 L87
           18615 S E2
                  E PROSTATE/CT
 L88
              26 S E3+OLD, NT
           32483 S E18+OLD, NT
 L89
 L90
           32840 S E53+OLD, NT, PFT, RT OR E57+OLD, NT, PFT, RT
                  E PITUITARY/CT
                  E E3+ALL
                  E E2+ALL
 L91
           41881 S E3+OLD, NT OR E15+OLD, NT
                  E MENINGIOMA/CT
                  E E3+ALL
L92
              668 S E2,E3
                  E UTERIN MYOMETRIAL FIBROID/CT
                  E UTERINE MYOMETRIAL FIBROID/CT
                 E MYOMETRIAL FIBROID/CT
                 E E5+ALL
 L93
            3124 S E2
                 E UTERINE FIBROID/CT
                 E FIBROID/CT
                  E E4+ALL
```

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L94
            722 S E2
L95
              3 S L29 AND L66-L94
L96
              9 S L60, L65, L95
                E UTERUS, NEOPLASM/CT
L97
          12762 S E3+OLD, NT
                E PROSTATE, NEOPLASM/CT
                E PROSTATIC NEOPLASM/CT
                E E4+ALL
L98
          19786 S E2+OLD,NT
                E PITUITARY NEOPLASM/CT
                E E3+ALL
L99
           3354 S E2+OLD, NT
                E BREAST, NEOPLASM/CT
                E BREAST NEOPLASM/CT
                E E3+ALL
L100
          47677 S E2+OLD, NT
                E OVARY, NEOPLASM/CT
L101
          14597 S E3+OLD, NT
                E COLON, NEOPLASM/CT
                E COLON NEOPLASM/CT
                E E4+ALL
          18615 S E2
L102
L103
              2 S L29 AND L97-L102
L104
              9 S L96,L103
                E CARCINOMA/CT
L105
         108005 S E3+OLD, NT
L106
              1 S L29 AND L105
                E ANTIPROGEST/CT
                E E4+ALL
L107
            344 S E1, E2
L108
              5 S L29 AND L107
L109
              9 S L104, L106, L108
L110
              9 S L30, L109
             11 S L29 AND (PD<=20020625 OR PRD<=20020625 OR AD<=20020625)
L111
L112
              7 S L110 AND L111
L113
              4 S L111 NOT L112
     FILE 'REGISTRY' ENTERED AT 07:51:16 ON 05 JUL 2005
L114
             11 S L23 AND NC4/ES
L115
              1 S L114 AND C16H15N3OS
     FILE 'HCAPLUS' ENTERED AT 07:53:31 ON 05 JUL 2005
L116
              5 S L115 OR TANAPROGET OR NSP989 OR NSP 989
              3 S L116 AND (PD<=20020625 OR PRD<=20020625 OR AD<=20020625)
1.117
L118
              9 S L116, L117, L112
L119
              9 S L118 AND L3-L12, L27-L113
     FILE 'REGISTRY' ENTERED AT 07:55:02 ON 05 JUL 2005
     FILE 'HCAPLUS' ENTERED AT 07:55:28 ON 05 JUL 2005
     FILE 'USPATFULL' ENTERED AT 07:56:32 ON 05 JUL 2005
L120
              5 S L116
L121
             10 S L23
L122
              8 S L24
L123
             10 S L120-L122
L124
              9 S L123 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L125
             10 S L123, L124
```

FILE 'USPATFULL' ENTERED AT 07:57:34 ON 05 JUL 2005

FILE 'REGISTRY' ENTERED AT 07:57:47 ON 05 JUL 2005

L126 76 S L123 NOT L115 L127 76 S L23 NOT L115

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